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MAGNETIC PROPERTIES OF ITINERANT ELECTRONS

I. FERROMAGNETISM

by

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ABSTRACT

We have here considered a gas of electrons with a positive background interacting among themselves through a bare Coulomb potential at $T = 0^\circ\text{K}$. On examining the single-particle states of the system, one discovers that the bare Coulomb potential is screened by a dynamic dielectric constant. The same screening is shown to appear also when the low-lying excitations of the spin-wave type involving particle-hole pairs are examined. Now, in the random phase approximation and in the static limit where the plasma effects are neglected and for long waves, this screening is the usual Thomas-Fermi screening. One may thus start with a Yukawa potential which contains an arbitrary screening. This has not only the advantage of taking into account

* This work was done when N.R. Ranganathan was visiting Brandeis University during 1961-1963. Chapter III, Cases (a) and (b) were formulated in collaboration with N. R. Ranganathan.

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some correlations but also includes the extreme long-range and the extreme short-range interactions as special cases. The coupling strength is then defined as proportional to the ratio of the exchange to the kinetic energy. These considerations motivate the use of the Yukawa potential for the present problem.

We compute the ground state energy of such a system in the Hartree-Fock approximation, but excluding for the moment the possibility of spin density waves. This energy is a function of coupling strength, screening ξ and relative magnetization ζ . Examining the absolute minimum of this energy as a function of magnetization for various coupling strengths and screening constants we find some interesting features. For $\xi \leq 0.9$ we find the ground state is either paramagnetic or ferromagnetic depending on the value of the coupling strength; for $\xi > 0.9$ the unsaturated ferromagnetic states also compete. For $\xi < 0.9$ the intermediate states are relative maxima and, hence, do not appear. The case where $\xi = 0$ is the Coulomb problem and was studied earlier by Bloch in 1929. For $\xi > 0.9$ and much larger tending to infinity, one has the extreme short-range model of Stoner (1938). The results obtained by us go over into this case smoothly. Thus, a kind of phase diagram is obtained which describes the various ground states as the screening and the coupling strengths are varied. It is interesting to point out that if the Thomas-Fermi value is used for the screening, it is found that the gas stays paramagnetic for all densities.

The spin wave excitations in the system are also considered within the context of the random phase approximation (RPA). The equation describing these is solved for long wavelengths of the spin wave. The existence of spin waves is clearly brought out by computing the coefficient of q^2 which is the first non-zero term in this expansion. This coefficient contains two terms with opposite signs. By demanding that the spin-wave frequency be positive, one may define the stability of the spin waves. The condition for this coincides with that obtained for the ferromagnetic case by Herring both for the Coulomb and for the Stoner gases when appropriate limits are taken. A consequence of this criterion is that if the ground state is a stable ferromagnetic state (i. e., stable with respect to individual particle excitations) then it is also stable with respect to collective spin-wave excitations in the long wave limit. There exists a maximum wave vector for the spin wave beyond which it is unstable, being scattered into individual particle states.

A matrix Green's function formalism is here developed to treat this problem. This formalism is a modification of Nambu's for superconductivity theory. The method is quite general and is here employed also to extend formally the results to electrons in periodic potentials (Bloch electrons). The same method is also used to derive the equations for the symmetry breaking solutions of the Overhauser spin density wave type.

In an epilogue, some objections to the use of Yukawa potentials are considered. Also, the various aspects of extensions of the problem, some of which are only formally developed in the report, are outlined.

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In another technical report we will discuss some of the questions concerning collective states in SDW systems and itinerant electron anti-ferromagnetism.

MAGNETIC PROPERTIES OF ITINERANT ELECTRONS

I. FERROMAGNETISM

by

A. K. Rajagopal, H. Brooks, and N. R. Ranganathan

I. MOTIVATION AND STATEMENT OF THE PROBLEM

1. General Introduction

There are essentially two basic models of ferromagnetism in solids, and all others may be considered as variations on these two themes. The Heisenberg [1] model is based on the assumption that: (1) the electrons are localized on atoms; (2) only a single electron configuration corresponding to one electron per atom need be considered; and (3) the interatomic exchange effects can be treated by introducing an interaction $-2J_{ij}\underline{S}_i \cdot \underline{S}_j$ between the electrons localized on the sites i and j . Here J_{ij} is an exchange integral, \underline{S}_i and \underline{S}_j are the spin operators corresponding to the electrons at the sites i and j . This model is particularly suited to the case of insulators and will not be discussed here. For a recent review of exchange in insulators, one may refer to Anderson [2]. The itinerant model, on the other hand, developed by Bloch [3], Stoner [4], and Slater [5], is based on the competition between the kinetic energy of the electrons in a band and electron exchange in the Hartree-Fock approximation (hereafter referred to as HF). This exchange may be thought of as arising primarily from the intra-atomic rather than inter-atomic exchange. There are two extreme models of exchange based on long-range Coulomb interactions between the electrons (which were considered by Bloch [3]) and on zero-range interaction. The latter is shown here to be equivalent to a Weiss field and such a model was examined by Stoner [4]

and Slater [5]. Various modifications of the itinerant and the localized schemes to fit ~~the~~ real solids may be found in the review articles by Brooks [6a, b] and Vonsovskii and Izyumov [7].

It may be surmised that in an itinerant theory, the system may become ferromagnetic only for a certain ratio of the exchange energy to the kinetic energy. This ratio may be thought of as a suitable strength parameter, which determines the magnetic behavior. In the next two sections a brief summary will be given of the results found in the literature on the ground-state properties and also the collective excitations of such systems.

2. Ground-State Properties

In order to describe the ground-state properties, the total energy of the system must be computed and its absolute minimum as a function of relative magnetization, ξ , must be examined. This cannot be done exactly. The results to be described are within the HF approximation. This consists in assuming that the system behaves as if it were composed of "quasi" particles which are effectively free despite interaction. Also, this approximation takes into account only the parallel spin correlations between the electrons. Neglect of antiparallel spin correlations tends to exaggerate the tendency towards ferromagnetism; that is, it overestimates the difference in interaction energy between parallel and antiparallel spins of the electrons. This difference tends to be minimized when the interactions are short range, and therefore, antiparallel spin correlations can, to some extent, be taken into account phenomenologically by introducing a short-range interaction between

quasi particles. Most of the calculations on the ferromagnetism of an electron gas disregard such correlations. It is only recently that the interactions have been taken into account more fully for the ordinary (nonmagnetic) electron gas. A description of the ground-state properties in HF and some recent attempts to take account of correlations will be given in the next two sub-sections. It will be assumed that the system of electrons has a positive background so as to keep the entire system electrically neutral. All the calculations pertain to $T = 0^\circ\text{K}$, although the formalism will be such that this restriction is not necessary.

A. Coulomb Interaction

Bloch [3] was the first to compute the total energy of an electron gas in a positive background at $T = 0^\circ\text{K}$ in the HF approximation, as a function of the relative magnetization, ξ . The coupling strength for this problem is r_s , which is the effective radius of the electron in units of the Bohr radius and is inversely proportional to the cube root of the density of the system. He showed that for low densities, corresponding to $r_s \gtrsim 5.45$, the gas becomes ferromagnetic. This follows when the energy of the ferromagnetic state ($\xi = 1$) is compared with that of the paramagnetic state ($\xi = 0$). A similar calculation was made by several other authors, notably Brillouin [8], Wohlfarth [9], Lidiard [10], Shimuzu [11], and, very recently, Fukuda [12]. All obtained the same result as Bloch. Shimuzu tried to take into account the electron correlations by including the plasma effects, but his analysis was inconclusive. Cooper [13] extended the Gell-mann and Brueckner [14]

analysis for the ordinary (nonmagnetic) electron gas to the present problem. He concluded that taking into account more interactions gives ferromagnetism for $r_s \gtrsim 4.85$. His method consisted in taking into account a certain infinite set of ring diagrams. The conclusion is that the electron gas with Coulomb interactions in HF becomes ferromagnetic at low densities and paramagnetic at high densities. None of the authors quoted above seems to have considered carefully the possibility of intermediate polarizations as ground states.

B. Short-Range Interaction

Stoner [4] and Slater [5] modified the Sommerfeld model of the metal by postulating a phenomenological internal magnetic field in order to describe the ferromagnetic interaction. The coupling strength in this case is the ratio of the internal magnetic field energy, $K\theta'$, to the Fermi energy, ϵ_F , $K\theta'/\epsilon_F$. They assumed that the internal Weiss field acting on each electron is the same, so that the up and down spin bands are displaced rigidly. Slater [5], however, took into account the actual density of states distribution instead of the free electron one. The second assumption in this theory is that the electrons in their separate bands obey Fermi-Dirac (FD) statistics. Such a system was shown to have a paramagnetic (P) ground state for $K\theta'/\epsilon_F < 2/3$, an unsaturated ferromagnetic state (UF, $0 < \zeta < 1$) for $2/3 < K\theta'/\epsilon_F < 2^{-1/3}$, and a ferromagnetic state (F) for $K\theta'/\epsilon_F > 2^{-1/3}$. Wohlfarth [15] has recently reviewed the present status of this model.

The outstanding assumptions, the existence of a Weiss field and the use of FD statistics, remained to be justified in this theory. The first was

attempted by Wohlfarth [9] and Lidiard [10] and the second by Bell [16]. Wohlfarth [9] and Lidiard [10] showed that the assumption of Stoner that the exchange energy is proportional to the square of the relative magnetization is not strictly true. More generally, it is given by a power series in ζ^2 ; the coefficients of this series involve certain overlap integrals. Earlier, Brooks [6b] had examined in detail the ground-state properties for such a generalized Weiss field. Bell [16] explicitly examined the statistics of the Weiss field and showed by a direct calculation of the partition function that the use of FD distributions for the up and down bands can be made consistent. This is achieved by summing, for each magnetic quantum number m , over the sets of occupation numbers which are consistent with that value of m . Recently, Suris [17] reformulated the Stoner problem using a Green's function method. He found that Stoner's model is equivalent to an electron gas interacting through a zero-range potential in the HF approximation. The FD distributions for the up and down spins follow as a natural consequence as does also the Weiss form of the exchange energy. Suris then reproduced the results derived by Stoner although his method of solution of the resulting integral equations was more analytical than was the case with Stoner's work. Thus, this model is shown to exhibit an F state for high densities, a P state for low densities and for the intermediate densities, UF states, in contrast to the behavior of the Coulomb gas.

All the above remarks concern the symmetry-preserving solutions of the HF equations. Recently, Overhauser [18] showed that there exist symmetry-breaking solutions of the HF equations which have lower energy than the usual solutions. In particular, he showed that in a Coulomb gas, the P state is

never the ground state. It is always unstable towards the formation of static spin-density wave (SDW) states. This has been confirmed by Fukuda [12]. In an electron gas with zero-range interaction, according to Overhauser, the SDW states do not occur as ground states at all, for any coupling strength or density. But Fukuda finds that these states are more stable than the P state for coupling strengths for which the UF is known to be stable.

3. Individual Particle and Collective Excitations

The low-lying excitations in a medium close to the ground state are equally important in the study of any system. In the Heisenberg model of a ferromagnet, besides the spin-aligned state constituting the ground state, there exist spin-wave states close to the ground state. The existence of spin waves in both ferromagnetic metals and insulators has been established experimentally [6a]. Originally, the existence of spin waves was proved theoretically by Bloch [19] only for the Heisenberg model. For quite some time, the absence of spin waves on an itinerant model was thought to be a serious drawback of the itinerant theory. Slater [20], however, demonstrated that taking into account interactions more fully would produce spin waves on such a model. This view was later amplified by Herring and Kittel [21] and by Herring [22, 23]. The first paper gave largely phenomenological arguments and a more rigorous development appeared in the subsequent papers. In an insulator one may describe the spin waves as follows. In the

ground state, the spins are all localized on the lattice sites of the insulator and are all lined up. The first excited state is such that one of the spins on one of the lattice sites is reversed and since the system has translational symmetry this propagates as a spin reversal mode. Herring and Kittel [21] gave arguments to show that, despite the fact that the electrons are wandering throughout the metal lattice, their spin motions are correlated because of the exclusion principle. They showed that an electron moving in a ferromagnetic metal is continually gyrate because the electrons in its immediate vicinity tend to align the spin of this electron with their average spin moment. So they postulate a phenomenological expression for the energy due to this torque involving a "Bloch wall coefficient" which is shown to be related to the spin-wave energy in the lowest order of perturbation theory. Herring [22, 23] treated this model in detail both for the Coulomb gas and for the short-range model. The approach was to treat the ferromagnetic material as a continuous medium in which the three components of spin density are regarded as the amplitudes of a vector field quantized in the way demanded by the known commutation rules for the spin components. They showed that there exist low-lying spin-wave states and that these are orthogonal to all the low-lying individual particle states of the usual itinerant electron model. This same picture is employed by all the subsequent authors including the present ones.

A. Coulomb Gas

Herring [22] computed the spin-wave frequency in the long wavelength limit for the ferromagnetic state, using the model proposed earlier [21]. For the Coulomb gas he found that the coefficient of q^2 (where q is the magnitude of the wave vector of the spin wave) consists of two terms. By demanding that the spin-wave frequency be positive, he derived a stability condition which showed that stable spin waves exist for $r_s > 5.485$. This is slightly larger than the value derived by Bloch [3] using the ground-state criterion ($r_s > 5.45$). Recently, Fukuda [12] rederived this result using an equation of motion technique in the random phase approximation (RPA) including exchange, also in the limit of small q . He obtained a value of $r_s > 5.145$. However, he made a numerical error in computing this value. The correct stability criterion is $r_s > 5.344$. This result seems more plausible than Herring's, since it implies that when r_s is large enough to make the ferromagnetic state stable with respect to individual particle excitations (essentially the Bloch criterion), then the criterion for spin-wave stability is automatically satisfied. In other words, the Bloch criterion is stronger than the spin-wave criterion, and as we shall see, this result also applies in the case of the general Yukawa interaction.

B. Short-Range Gas

Herring [23] also computed the spin-wave energy in the long wave limit for the ferromagnetic state using the short-range model. He computed the coefficient of q^2 as in the Coulomb case and found that the spin-wave stability condition is $K\theta'/\epsilon_F > 2^{5/3}/5 = 0.635$. The required coupling is smaller than that required for stability of the complete F state ($K\theta'/\epsilon_F > 0.794$) or for that matter, the criterion for the UF state ($K\theta'/\epsilon_F > 0.667$). The same result is also derived by Fukuda [12]. This implies that the spin waves are stable whenever either UF or F state is a stable ground state. Besides finding the spin waves, Herring and Kittel [21] had given arguments to show that there are other excited states which are of the Stoner type particle-hole pair scattering states. These were shown to be orthogonal to the spin-wave states. Hereafter, we shall refer to the spin-wave states as "bound states" since they are states of lower total spin polarization than the ground state but lying lower in energy than the lowest excited individual particle states corresponding to the transfer of one electron of one spin distribution to the other. Thompson [24] has recently proposed an extension of the usual determinantal method for treating the ferromagnetic metal. His work is very close in spirit to that of Herring. He considered only the short-range interaction model. His calculation is more general than Herring's in that he computed the spin-wave dispersion law for the F state for arbitrary q . Besides rederiving Herring's expression for the coefficient of q^2 , he showed that the spin waves become degenerate with the single particle excitations of the Stoner

type above a certain q_{\max} . This is shown schematically in Fig. 1a. This degeneracy actually results in the breaking up of the bound state into the scattering states. The spin wave decays by carrying an up spin electron into a spin down state, and energy and momentum must be conserved in this process. The difference in energy of the up and down electrons is finite as shown in Fig. 1a, and the momenta must be such that the up electron must be inside the up Fermi sphere while the down electron must be outside the down Fermi sphere. With these restrictions, for small q , this process is energetically impossible while for a certain q_{\max} and beyond it is indeed possible. This process can take place for all suitable momenta of the electrons satisfying these conditions and, hence, one gets a continuum of scattering states as shown in the figures. The bounding curves are for the electrons near the Fermi sphere. If the calculation is followed carefully, it is seen that a lifetime appears for the bound state as soon as it reaches the continuum of scattering states. The interesting feature is that for $\zeta < 1$, the gap at $q = 0$, $2K\theta'\zeta$, decreases and so for the UF states the q_{\max} is bound to be smaller than that for the F state and finally for $\zeta = 0$, the P state, there are no bound spin-wave states. This picture is essentially the same for the Coulomb case also.

Edwards [25] tried to extend and generalize Herring's work for Bloch states but did not report any explicit calculations. He derived an improved version of the general expressions for the spin-wave dispersion in the long wavelength limit using diagrammatic techniques for the evaluation of matrix elements. He also indicated how the coefficients of higher powers in q

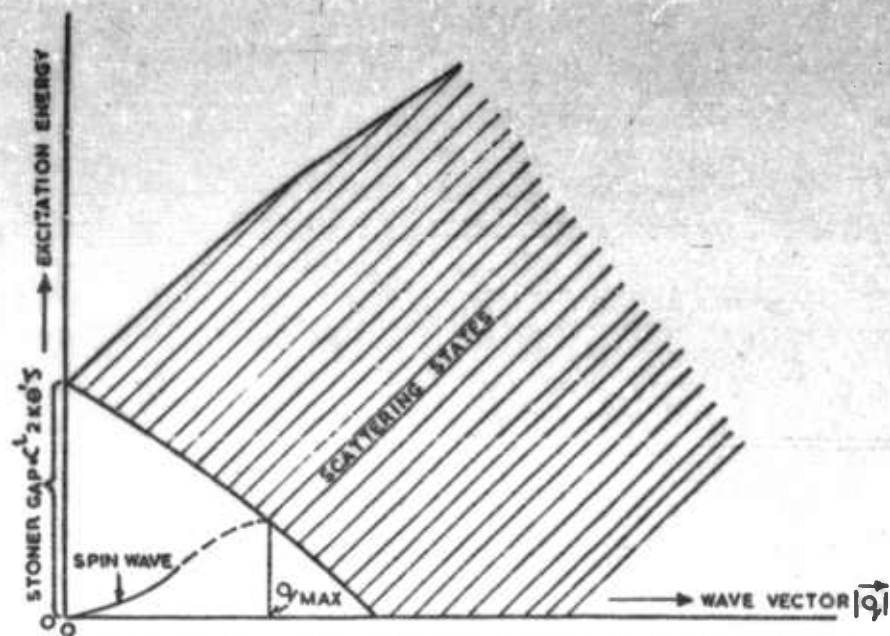


FIG.1a: DISPOSITION OF SCATTERING STATES AND THE COLLECTIVE MODE IN \uparrow_{-} (SCHEMATIC)

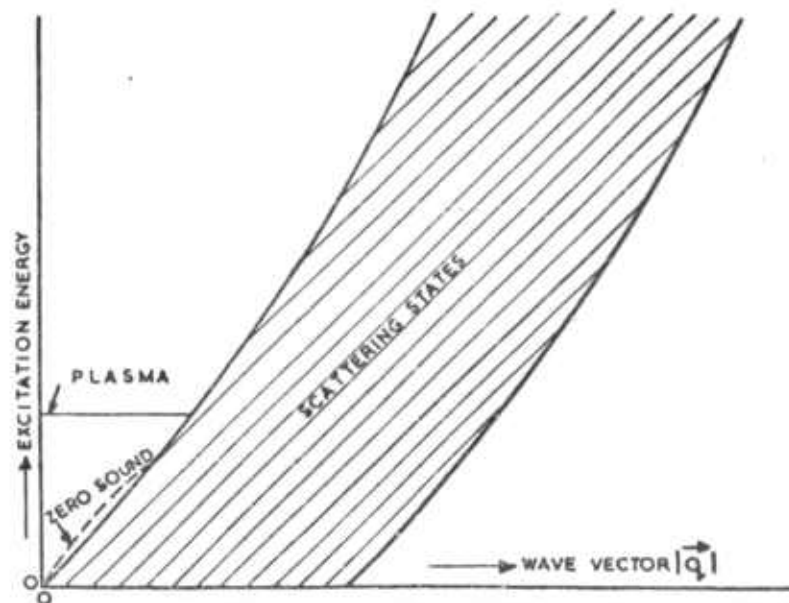


FIG.1b: DISPOSITION OF SCATTERING STATES AND THE COLLECTIVE MODE IN γ_0 (SCHEMATIC)

could be calculated. Kubo, et al. [26], using a Green's function technique, treated the short-range itinerant electron model in RPA including exchange. These authors were interested in computing the spin-wave contribution to the neutron scattering for an itinerant electron ferromagnetic system. Such a model was shown to be capable of accounting for the observed diffuse scattering. In this calculation it is necessary to compute the dynamical susceptibilities. The spin-wave dispersion so derived agrees with Thompson's [24]. Baym [27], using a Boltzmann equation technique, derived the same results for the same model. He also gave arguments like Thompson's for the spin-wave states strongly mixing with the individual particle states above a certain wave vector. It is also of interest that, using the Landau theory of Fermi liquids as a model for the electrons in a metal, Abrikosov, et al. [28], showed the possibility of spin waves in a ferromagnetic metal. Antonoff [29], using an equation of motion method, also attempted this problem; he employed what he called a "degenerate kernel approximation," besides RPA, and obtained spin waves. He also computed the maximum wave vector q_{\max} as was done by Thompson and Baym. Fukuda [12] has examined the problem of spin waves based on the Stoner model but he only computed the spin-wave frequency in the long wavelength limit and in the ferromagnetic state like all others. Thus several authors have computed the spin-wave frequency in the long wavelength limit and for the F state for the Stoner model. It must be added that Kubo, et al., and Baym (loc. cit.) found zero sound type collective oscillations to exist, also. These results are summarized in Table 1.

TABLE 1: Individual Particle and Collective Excitations
(Stoner Gas)

<u>Type of Disturbance</u>	<u>Collective Mode</u>	<u>Scattering States</u>	<u>P State</u>
density-density	$\omega \sim q$ } (zero sound)	$\left\{ \begin{array}{l} \omega = E_{\sigma}(k+q) - E_{\sigma}(k) \\ (\sigma = \uparrow, \downarrow) \end{array} \right.$	(zero sound)
long. spin susc.	$\omega \sim q$ }		
trans. spin susc.	$\omega \sim q^2$ (spin wave)	$\omega = E_{\sigma}(k+q) - E_{\sigma}(k)$ } no resonant response	

$$E_{\sigma}(k) = k^2/2m - \bar{v}N_{\sigma} \quad (N_{\sigma} = k_{F\sigma}^3/6\pi^2)$$

$k_{F\sigma}$ = radius of σ -Fermi sphere, \bar{v} : interaction potential.

The density-density response function, longitudinal, and transverse spin susceptibilities may be thought of as describing, respectively, the spin singlet and the spin triplet with projections 0 and 1 of the particle-hole pairs. The scattering states for the density response function and the longitudinal spin susceptibility are of the form shown in the schematic sketch, Fig. 1b. Here the zero-sound mode is seen to be quite close to the scattering states. The plasma state is shown in this same figure, anticipating the future discussion of the Coulomb gas. The absence of an energy gap in the excitation spectra must be noted.

It is interesting to compare the corresponding results for the P state when the interaction is taken to be of zero range. Here only zero sound appears in the density response while no resonant responses appear in the susceptibilities as might be expected. In this limit the results are well known.

(Zero sound: Gottfried and Picman [30] and spin susceptibility: Wolff [31]). The corresponding calculations for the Coulomb gas are not found in the literature.

4. Present Work

From the brief summary of the previous work in the last two sections, it is clear that the itinerant electron model of ferromagnetism has recently seen a revival of interest. The conclusions of Bloch [3] and subsequent authors on the Coulomb gas were slightly obscured because the absolute minimum of the ground state was not carefully examined. For the P state, much work on the many-body aspects has been accomplished using modern field-theory techniques. For a recent review of this one may refer to the books of Pines [32, 33] and Anderson [34]. Shimuzu [11] used the Bohm-Pines method to examine the many-body effects on the criterion for ferromagnetism. His results were inconclusive because he did not examine the total energy as a function of magnetization. Except for the work of Cooper [13], the extension of field theoretic methods to the ferromagnetic problem has not been carried out and even this work is not without objections. One of the main objections to Cooper's work, as he himself realizes, is that the ring diagrams that were summed are valid only for high density ($r_s < 1$) and the second major objection is that he only compared as Bloch did, the F and P energies.

It has often been suggested in the literature, notably by Lidiard [10] and Wohlfarth [35], that some account of correlations can be included by using a Yukawa potential for the interaction. This contains a screening

parameter and, hence, includes both the extreme long-range Coulomb case and the extreme short-range Stoner case as limits. The suggestion actually came from Landsberg [36] who tried to explain the soft x-ray emission bands of sodium on a Sommerfeld model of the metal. Very recently, Robinson et. al., [37], considered the justification, within the context of RPA, of the use of such a Yukawa potential for nonmagnetic problems. The screening can be shown to come about when particle interactions are taken into account. Pines [38] had earlier shown that taking into account the electron-electron interaction brings about a screened interaction between electrons, of range k_c^{-1} (in his notation). He showed, even though this has a very different structure, that it resembles the Yukawa potential quite closely up to distances comparable to or less than k_c^{-1} . All these arguments pertain to the nonmagnetic case. Whatever be the consideration for the use of Yukawa potential in an interacting system, it seems fruitful to re-examine the problem afresh as the behavior of the Coulomb and the Stoner gases are completely different. The Yukawa potential may give an insight into the effect of range on the criterion of ferromagnetism.

The use of the Yukawa potential may be justified for the magnetic problem in much the same way as was done by Robinson, et al. [37]. If, in an interacting electron gas, the behavior of a single electron is examined, it is seen that even though one starts with a bare Coulomb interaction the exchange is screened in general by the dynamic dielectric constant. In the RPA, and if plasma effects are neglected by assuming the dielectric constant to be static, and working in the long wavelength limit, it is found that the

interaction potential has now the appearance of a Yukawa potential with the screening parameter given by the familiar Thomas-Fermi screening. This same screening can be shown to appear when the collective excitations of the spin-wave type are examined. In this way, the use of the Yukawa potential may be justified. This will be amplified in later chapters.

The Green's function method is employed here as it is found to be powerful enough to include all the results of previous authors and also to extend them, as will be indicated in subsequent sections. Thus a unification of all the results both as to the nature of the interactions and as to the use of a unified and elegant technique for attacking the present problem is here attempted. All the previous authors concerned themselves with plane waves while the present work indicates extensions to Bloch waves also.

Besides making a more complete study of the ground state of a polarized gas, the few non-rigorous attempts of Wohlfarth [15], Lidiard [10], and Bell [16] to justify the use of a Weiss field and FD distributions will be here given a more satisfactory justification. This consists in showing that a quasi-particle picture is valid in metals as was done by Luttinger [39] for the ordinary interacting electron gas, whereas the authors quoted above could only show the consistency of such assumptions. They could prove that the exchange energy is in general a power series in ξ^2 . Here it is seen to be a complicated function of ξ^2 , and so the convergence becomes slower as ξ^2 approaches unity. Bell showed how the partition function could be correctly evaluated in the presence of a Weiss field and, hence, also established

the validity of the FD distributions for the particle. These fall out automatically in the present approach.

On the collective aspects of the system, most of the authors confined themselves to the short-range Stoner model and the F state. For completeness the Coulomb gas must also be studied in the same spirit. This problem is much harder. In the present work the spin waves are studied in detail in the long wave limit and a formal power series expansion is also given for the frequency of the spin wave. Herring's [22, 23] method, though ingenious, is valid only in the long wave limit. He used a perturbation method for the HF equations and from the agreement with the present work, this may be viewed as RPA in a different form. Thompson's [24] determinantal method is very cumbersome. The method of Edwards [25] gives a technique for evaluating the coefficients of various powers of q and, hence, is also quite cumbersome. The method of Kubo, et al. [26], uses a factorization of the Green's functions which is equivalent to RPA, and this is here rederived. Baym's [27] Boltzmann equation technique is equivalent to RPA right from the start and it is hard to see the complete equation before the approximations are made. Antonoff's [29] method is similar to that of Kubo, et al.; his use of the "degenerate kernel" approximation may be shown to be equivalent to the localization of the spins, with a Heisenberg-type interaction. This invalidates the purpose of a fully itinerant theory. The same objection is also applicable to the work of Shimuzu [11], who explicitly assumes in an ad hoc fashion a Heisenberg-type interaction between the electrons.

Thus, it is seen that there is only a sketchy account of the polarized gas using field theory techniques in the literature. There is thus scope for further generalization of the problem in that one could include the results found in the literature as special cases of the Yukawa potential.

A. Ground-State Properties

The ground-state energy of a system of electrons in a positive background in HF approximation at $T = 0^\circ\text{K}$ is here computed as a function of ζ ($0 \leq \zeta \leq 1$) when the electrons are interacting through a Yukawa potential. The problem is studied in detail as a function of screening (ξ), magnetization (ζ) and density (ar_g). To determine the ground state, the absolute minimum of the total energy as a function of ζ for various ar_g and ξ is studied. It is found that for ξ much smaller than the diameter of the ferromagnetic Fermi sphere, the system behaves essentially like the long-range Coulomb system. It is found in this case that the F state is the ground state for low densities and the P state for high densities. The UF states can never lie lowest as they are relative maxima. This indicates why the comparison of just the energies of F and P states in the Coulomb case is sufficient. For ξ much larger than the diameter of the ferromagnetic Fermi sphere, the gas behaves like the short-range Stoner gas with all the three states of magnetization having the possibility of being the ground state. This difference in the behavior comes about because of the different forms the exchange energy takes in these two limits. In this connection, it may be mentioned that Brooks [6b], using a generalized Weiss field model

consisting of a power series in ξ^2 of the exchange energy (cf. Wohlfarth [15]) had shown that the UF states cannot be ground states if the ratio of the coefficient of ξ^4 to that of ξ^2 exceeds a certain critical value. This observation had escaped the notice of Wohlfarth (loc. cit.) who did not examine the consequences of the generalized Weiss field. The parameter corresponding to Brooks's here is the screening. It is clear from the present analysis that as ξ increases the criterion for the F state changes abruptly beyond a certain critical value.

These results are summarized in Fig. 2a, b. Here a plot of the coupling strength ($\ln(\alpha r_g)$ in Fig. 2a and $K\theta'/\epsilon_F$ in Fig. 2b) against ξ is presented. This clearly shows that for $\xi \lesssim 0.9$ the nature of the ground state changes. A more detailed description will be given in Section II. The possibility of SDW being ground states has not been examined here for the Yukawa gas. From the work of Overhauser it is known that the ground state is an SDW state for densities at which the present theory shows the P state to be lowest.

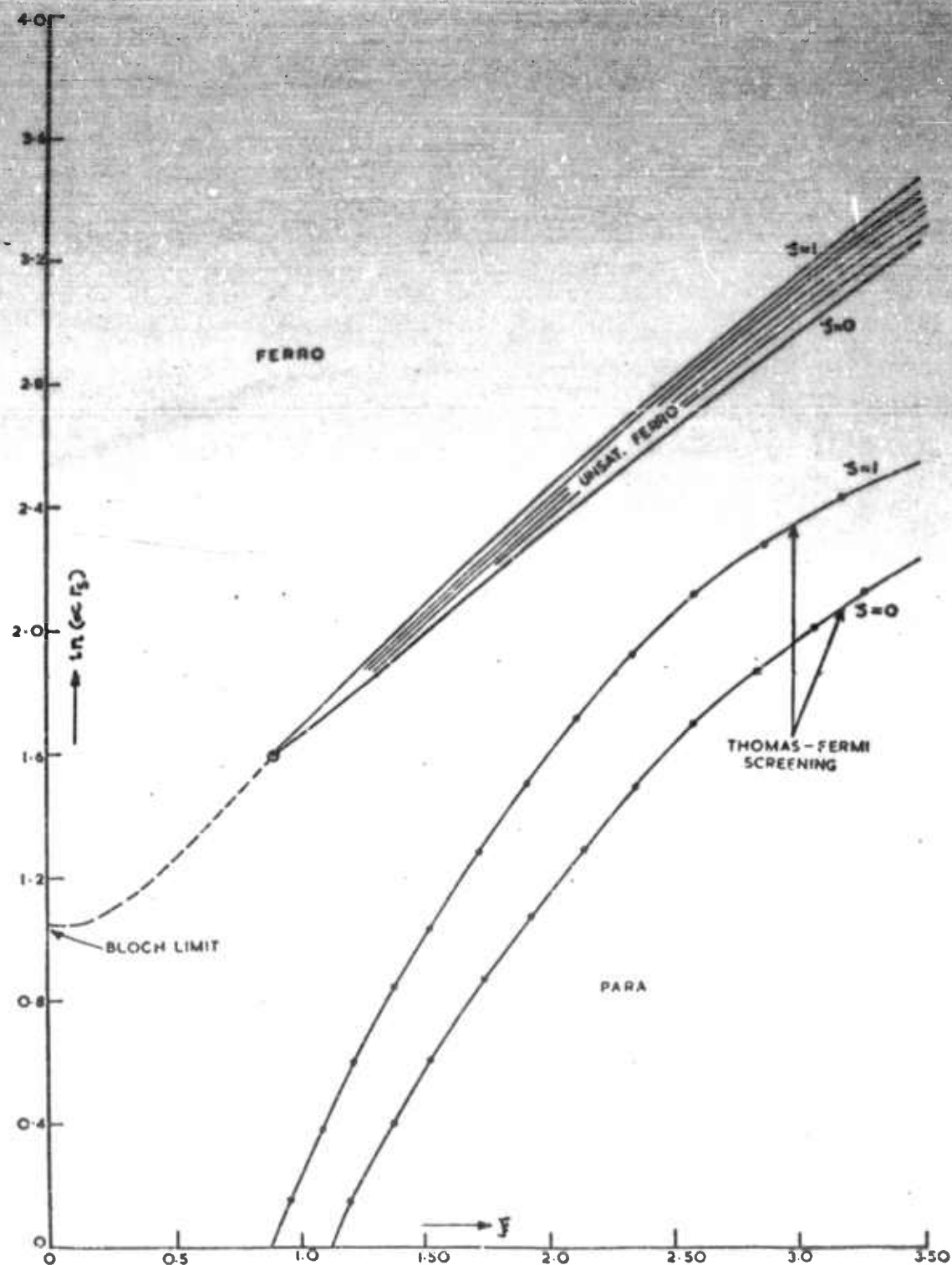


FIG. 2Q: PLOT OF COUPLING STRENGTH VS SCREENING (COULOMB)

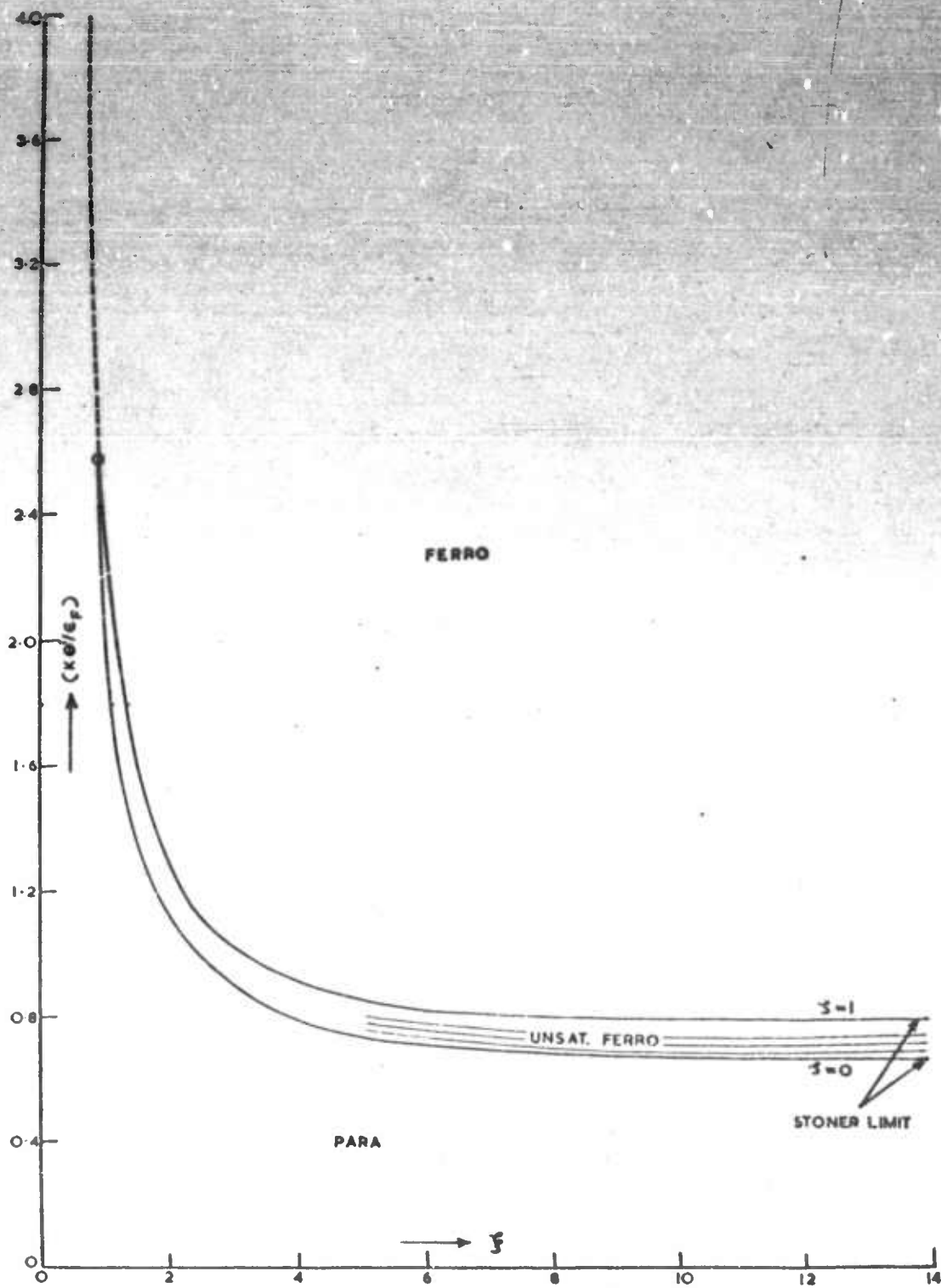


FIG. 2.6: PLOT OF COUPLING STRENGTH VS SCREENING (STONER)

B. Collective States

For $\xi = 0$ we have the Coulomb gas. In this case it is found that the density response in RPA with the exchange contribution completely neglected shows plasma resonance. When the exchange is neglected the medium behaves as though it consisted of two noninteracting electron gases with different effective masses. This is shown in Table 2. The transverse spin susceptibility also fails to show spin waves when exchange is omitted; however, the

TABLE 2: Individual Particle and Collective Excitations
(The Coulomb Gas)

<u>Type of Disturbance</u>	<u>Collective Mode</u>	<u>Scattering States</u>	<u>P State</u>
density-density	$\left. \begin{array}{l} \omega \sim \omega_{Pl} \\ \omega \sim \omega_{Pl} \\ [\omega \sim q^2 \text{ (spin wave)}] \end{array} \right\}$	$\omega = E_{\sigma}(k+q) - E_{\sigma}(k)$	$\omega \sim \omega_{Pl}$
long. spin susc.		$(\sigma = \uparrow, \downarrow)$	no resonant response
trans. spin susc.		$\omega = E_{\sigma}(k+q) - E_{-\sigma}(k)$	

$$E_{\sigma}(k) = k^2/2m - e^2/\pi k \left[k k_{F\sigma} + \frac{1}{2} (k^2 - k_{F\sigma}^2) \ln \left| \frac{k - k_{F\sigma}}{k + k_{F\sigma}} \right| \right]$$

$k_{F\sigma}$: radius of σ Fermi sphere; for small k ,

$$E_{\sigma}(k) \sim k^2/2m_{\sigma} - \frac{2e^2}{\pi} k_{F\sigma}; \quad \frac{1}{m_{\sigma}} = \left(\frac{1}{m} + \frac{4e^2}{3\pi k_{F\sigma}} \right).$$

equation describing it when exchange is included can be solved in the long wave limit. It is for this reason that in Table 2 the spin waves are shown within brackets. This was also done by Fukuda [12]. The method of Fukuda is used here and it is found that he made an error in the computation of the coefficient of q^2 ; he found in the F state, $\omega_{SW} \sim (q^2/2m)(1 - 5.145/r_s)$ whereas it is shown here that to the same order of approximation as Fukuda $\omega_{SW} \sim (q^2/2m)(1 - 5.344/r_s)$. This result must be compared with that derived by Herring [22]: $\omega_{SW} \sim (q^2/2m)(1 - 5.485/r_s)$.

For the sake of completeness the results for the P state are also given in the Table. Here only the plasma mode exists when exchange is neglected and there are no other excitations. The way the scattering states and the bound states are disposed is similar to that given earlier in the section on the short-range gas.

In the Yukawa case, the most interesting collective mode is the spin flip mode, after including exchange contributions. For any ξ , and for small q , by using the same technique as Fukuda, the coefficient of q^2 can be determined. For the F state, for $\xi = 0$ (Coulomb) and for $\xi \rightarrow \infty$ (short range), this goes over to the results obtained earlier. In the short-range case, a general dispersion law for spin waves of all q , and any magnetization ξ , (at $T = 0^\circ K$) is obtained. The coefficient of q^2 for the UF state is here derived. For the F state, this goes over to the result of Herring [23]. Also, the spin waves merge into the scattering states, which are of Stoner type, at about $3/4$ the F state Fermi momentum and the spin-

wave energy at this value of the wave vector is about $1/16$ of the F state Fermi energy. Similar estimates were made by Thompson for the F state and by Baym for the UF states (loc. cit.). In the UF state, the spin waves are stable for $K\theta'/\epsilon_F > (1/5) \left[\frac{(1+\xi)^{5/3} - (1-\xi)^{5/3}}{\xi} \right]$ whereas the Stoner condition is $K\theta'/\epsilon_F = (1/2) \left[\frac{(1+\xi)^{2/3} - (1-\xi)^{2/3}}{\xi} \right]$. Thus it is seen that the spin wave stability condition is always weaker than the Stoner condition. Also the q_{\max} for the UF states becomes smaller as ξ decreases as described earlier.

The formalism given here can be modified to treat the Overhauser [18] problem of the SDW states. We have rederived the Overhauser integral equations by our method in a straightforward manner. The extension to the Bloch states is also indicated here. The collective excitations of the plasma type for the Bloch electron system in the unpolarized case were first derived by Ehrenreich and Cohen [40] who used an equation of motion method. This is here generalized to the polarized case. The other response functions, namely the longitudinal and transverse spin susceptibilities are also computed for the Bloch scheme. The possibility of the existence of spin waves in the Bloch scheme could only be indicated in certain crude approximations due to the very complicated nature of the equations describing them.

In summary, the Yukawa gas behaves like a Coulomb gas for $\xi < 0.9$ with no UF states and for $\xi > 0.9$, like the Stoner gas, as displayed in

Figs. 2a, b. Also spin waves are present on such a model, and the coefficient of q^2 for the spin-wave frequency is computed. The results go over into those derived by Herring for the Coulomb and Stoner cases when appropriate limits are taken (with some modifications for the Coulomb case). It is shown that whenever the HF ground state is an F state, it also exhibits stable spin-wave excitations. In the Stoner gas, the spin waves for the F state are stable when the ground state is the UF state. Also, it is shown that there exists a q_{\max} for the spin waves at which they merge with the scattering states. This q_{\max} for the spin waves decreases as one decreases ξ . The scattering states are the usual Stoner-type excitations.

ARPA-11 II. SINGLE PARTICLE EXCITATIONS AND THE GROUND-STATE PROPERTIES

1. Introduction

After establishing the notation briefly, a discussion of the single particle states of the system under consideration will be given. The notation will be for the most part that of Martin and Schwinger [41] or equivalently Kadanoff and Baym [42]; the latter will be henceforth referred to as KB. For the sake of completeness a brief summary of Chapters 1, 2, and 5 of KB will now be given.

The quantum mechanics of a system of identical particles are best described in terms of second quantized operators, namely the creation operator $\psi_{\sigma_1}^{\dagger}(r_1, t_1)$ and the annihilation operator $\psi_{\sigma_1}(r_1, t_1)$ (when acting to the right). Here σ_1 stands for the spin orientation and (r_1, t_1) represent the space-time point, which will be represented in the future by 1. The dynamics of the system is described by

$$H = \sum_{\sigma} \int d^3r \psi_{\sigma}^{\dagger}(rt) \left[-\frac{\nabla^2}{2m} + V(r) \right] \psi_{\sigma}(rt) \\ + \frac{1}{2} \sum_{\sigma\sigma'} \iint d^3r d^3r' dt' \psi_{\sigma}^{\dagger}(rt) \psi_{\sigma'}^{\dagger}(r't') \mathcal{V}(r-r'; t-t') \psi_{\sigma'}(r't') \psi_{\sigma}(rt) \quad (2.1.1)$$

in units where $\hbar = 1$. Here the first term represents the kinetic energy, the second term, the single particle potential, and the last term represents the two-particle interaction potential between the particles. The interaction potential is taken to be instantaneous so that

$$\mathcal{V}(r-r'; t-t') = \mathcal{V}(r-r') \delta(t-t') \quad (2.1.2)$$

We will henceforth write $t^{\pm} = t \pm 0$; $G(rt; r't^{\pm}) = G(rr'; 0^{\pm}) = G(11^{\pm})$.

$\mathcal{V}(r-r')$ is normally the Coulomb potential and it is left unspecified for the present so as to preserve maximum generality. Since we are considering an electron system, the Pauli exclusion principle is written in the form of a set of anti-commutation rules at equal times for these operators:

$$[\psi_{\sigma}^{\dagger}(rt), \psi_{\sigma'}^{\dagger}(r't)]_{+} = 0; [\psi_{\sigma}(rt), \psi_{\sigma'}^{\dagger}(r't)]_{+} = \delta_{\sigma\sigma'} \delta^{(3)}(r-r') \quad (2.1.3)$$

where $[A, B]_{+} = AB + BA$. The equation of motion for any operator $X(t)$ in the Heisenberg representation is

$$i \frac{\partial X(t)}{\partial t} = [X(t), H]_{-} \quad (2.1.4)$$

where $[A, B]_{-} = AB - BA$. In order to study the thermodynamics of the system the grand canonical ensemble average is defined by

$$\langle X \rangle = \text{Tr} \{ e^{-\beta(H-\mu N)} X \} / \text{Tr} \{ e^{-\beta(H-\mu N)} \} \quad (2.1.5)$$

Here Tr stands for the trace on the states of the system; H is the total Hamiltonian and N is the number operator $\int \psi^{\dagger}(rt) \psi(rt) d^3r$, μ is the chemical potential and β is $1/KT$ with K , the Boltzmann constant and T the temperature on the absolute scale.

We now define single particle correlation functions

$$\left. \begin{aligned} G_{\sigma\sigma'}^{>}(11') &= \frac{1}{i} \langle \psi_{\sigma}(1) \psi_{\sigma'}^{\dagger}(1') \rangle \\ G_{\sigma\sigma'}^{<}(11') &= \frac{-1}{i} \langle \psi_{\sigma'}^{\dagger}(1') \psi_{\sigma}(1) \rangle \end{aligned} \right\} \quad (2.1.6)$$

These are respectively defined for $t_1 > t_1'$ and $t_1 < t_1'$, and for real times.

These functions define the propagation of disturbances in which a single

particle is added to the system at some space-time point 1 and removed at 1' in the first case while the second defines the opposite order of operations.

The single particle Green's function may be defined as

$$G_{\sigma\sigma'}(11') = \frac{1}{i} \langle T(\psi_{\sigma}(1) \psi_{\sigma'}^{\dagger}(1')) \rangle \quad (2.1.7)$$

where T is the Wick time ordering symbol for Fermions in the present case

$$\left. \begin{aligned} T(\psi_{\sigma}(1) \psi_{\sigma'}^{\dagger}(1')) &= \psi_{\sigma}(1) \psi_{\sigma'}^{\dagger}(1') \text{ for } t_1 > t_{1'} \\ &= -\psi_{\sigma'}^{\dagger}(1') \psi_{\sigma}(1) \text{ for } t_1 < t_{1'} \end{aligned} \right\} \quad (2.1.8)$$

It follows that

$$\begin{aligned} G_{\sigma\sigma'}(11') &= G_{\sigma\sigma'}^{>}(11') \text{ for } t_1 > t_{1'} \\ &= G_{\sigma\sigma'}^{<}(11') \text{ for } t_1 < t_{1'} \end{aligned}$$

All the above definitions hold for real time domains. Using the equation of motion for $\psi_{\sigma}(1)$, the equation for $G_{\sigma_1\sigma_2}(12)$ may be constructed. Before discussing this, a few general remarks about G will now be made which follow by virtue of its definition. Now formally, since $\text{Tr}(ABC) = \text{Tr}(BCA) = \text{Tr}(CAB)$, one has a relation between $G^{>}$ and $G^{<}$ at the boundaries of an imaginary time domain

$$G_{\sigma\sigma'}^{<}(11')|_{t_1=0} = -e^{\beta\mu} G_{\sigma\sigma'}^{>}(11')|_{t_1=-i\beta} \quad (2.1.9)$$

Or, if the domain of definition of G is extended to imaginary times $0 < it < \beta$, one may write formally

$$G_{\sigma\sigma'}(11')|_{t_1=0} = -e^{\beta\mu} G_{\sigma\sigma'}(11')|_{t_1=-i\beta} \quad (2.1.10)$$

along with

$$\begin{aligned} G_{\sigma\sigma'}(11') &= G_{\sigma\sigma'}^{>}(11') \text{ for } it_1 > it_1', \\ &= G_{\sigma\sigma'}^{<}(11') \text{ for } it_1 < it_1'. \end{aligned}$$

These may be written equivalently in the other time variable also. Since the system under consideration has time translational invariance, the functions $G^{>}$, $G^{<}$, G are functions of the difference $(t_1 - t_1')$ only. In view of this, (2.1.9) may be written as

$$\begin{aligned} G_{\sigma\sigma'}^{<}(r_1 r_1'; t) &= -e^{\beta\mu} G_{\sigma\sigma'}^{>}(r_1 r_1'; t-i\beta) \\ &\quad (0 \leq t \leq \beta) \end{aligned} \tag{2.1.11}$$

Now the Fourier transforms in time may be introduced:

$$\begin{aligned} G_{\sigma_1\sigma_2}^{>}(r_1 r_2; \omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} G_{\sigma_1\sigma_2}^{>}(r_1 r_2; t) \\ G_{\sigma_1\sigma_2}^{<}(r_1 r_2; \omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} G_{\sigma_1\sigma_2}^{<}(r_1 r_2; t) \end{aligned}$$

(KB use a factor i in the first, and $-i$ in the second relation). Using (2.1.11)

$$G_{\sigma_1\sigma_2}^{<}(r_1 r_2; \omega) = -e^{\beta\mu} \int_{-\infty}^{\infty} dt e^{i\omega t} G_{\sigma_1\sigma_2}^{>}(r_1 r_2; t-i\beta)$$

so that formally one gets

$$G_{\sigma_1 \sigma_2}^{<}(r_1 r_2; \omega) = -e^{-\beta(\omega - \mu)} G_{\sigma_1 \sigma_2}^{>}(r_1 r_2; \omega). \quad (2.1.12)$$

We now introduce the spectral weight function $A_{\sigma_1 \sigma_2}(r_1 r_2; \omega)$:

$$A_{\sigma_1 \sigma_2}(r_1 r_2; \omega) = G_{\sigma_1 \sigma_2}^{>}(r_1 r_2; \omega) - G_{\sigma_1 \sigma_2}^{<}(r_1 r_2; \omega). \quad (2.1.13)$$

Clearly, then

$$\left. \begin{aligned} G_{\sigma_1 \sigma_2}^{>}(r_1 r_2; \omega) &= (1 - n_F(\omega)) A_{\sigma_1 \sigma_2}(r_1 r_2; \omega) \\ G_{\sigma_1 \sigma_2}^{<}(r_1 r_2; \omega) &= -n_F(\omega) A_{\sigma_1 \sigma_2}(r_1 r_2; \omega) \end{aligned} \right\} \quad (2.1.14)$$

where $n_F(\omega) = 1/(\exp(\omega - \mu)\beta + 1)$.

One may write a Fourier series representation of $G_{\sigma_1 \sigma_2}(1, 2)$ in view of (2.1.10) (Chapter 3 of KB, Pp 19, 20)

$$G_{\sigma_1 \sigma_2}(r_1 r_2; t_1 - t_2) = \left(\frac{1}{-i\beta} \right) \sum_{\nu \text{ (odd integers)}} e^{-iz_{\nu}(t_1 - t_2)} G_{\sigma_1 \sigma_2}(r_1 r_2; z_{\nu}) \quad (0 \leq it_1, it_2 \leq \beta) \quad (2.1.15)$$

where $z_{\nu} = (\pi \nu / -i\beta) + \mu$. Since the condition (2.1.10) holds for both the time variables, the Fourier coefficient is given by

$$G_{\sigma_1 \sigma_2}(r_1 r_2; z_{\nu}) = \int_0^{-i\beta} e^{+iz_{\nu}(t_1 - t_2)} G_{\sigma_1 \sigma_2}(r_1 r_2; t_1 - t_2) dt_1.$$

This must, however, be independent of t_2 and letting $t_2 \rightarrow 0^+$, so that

$$G_{\sigma_1 \sigma_2}(r_1 r_2; z_v) = \int_0^{-i\beta} dt_1 e^{+iz_v t_1} G_{\sigma_1 \sigma_2}^>(r_1 r_2; t_1).$$

But

$$G_{\sigma_1 \sigma_2}^>(r_1 r_2; t_1) = \int \frac{d\omega}{2\pi} e^{-i\omega t_1} A_{\sigma_1 \sigma_2}(r_1 r_2; \omega) / (1 + e^{-(\omega - \mu)\beta})$$

and, hence, after some manipulation,

$$G_{\sigma_1 \sigma_2}(r_1 r_2; z_v) = \int \frac{d\omega}{2\pi i} \frac{A_{\sigma_1 \sigma_2}(r_1 r_2; \omega)}{\omega - z_v}. \quad (2.1.16)$$

Thus, the Fourier coefficient is just an analytic function

$$G_{\sigma_1 \sigma_2}(r_1 r_2; z) = \int \frac{d\omega}{2\pi i} \frac{A_{\sigma_1 \sigma_2}(r_1 r_2; \omega)}{\omega - z}$$

evaluated at $z = z_v$, provided A has no other singularities. A careful analysis of this analytic continuation is given in KB. It is obvious that

$$A_{\sigma_1 \sigma_2}(r_1 r_2; \omega) = \lim_{\epsilon \rightarrow 0} [G_{\sigma_1 \sigma_2}(r_1 r_2; \omega + i\epsilon) - G_{\sigma_1 \sigma_2}(r_1 r_2; \omega - i\epsilon)]. \quad (2.1.17)$$

This immediately leads to the sum rule

$$\begin{aligned} \int \frac{d\omega}{2\pi i} A_{\sigma_1 \sigma_2}(r_1 r_2; \omega) &= \lim_{\epsilon \rightarrow 0} \int \frac{d\omega}{2\pi i} [G_{\sigma_1 \sigma_2}(r_1 r_2; \omega + i\epsilon) - G_{\sigma_1 \sigma_2}(r_1 r_2; \omega - i\epsilon)] \\ &= \delta_{\sigma_1 \sigma_2} \delta^{(3)}(r_1 - r_2) \end{aligned} \quad (2.1.18)$$

because

$$i [G_{\sigma_1 \sigma_2}(x_1 x_2; 0^+) - G_{\sigma_1 \sigma_2}(x_1 x_2; 0^-)] = \delta_{\sigma_1 \sigma_2} \delta^{(3)}(r_1 - r_2)$$

which is the canonical commutation rule at equal times. The advanced and the retarded Green's functions could equally well have been introduced

$$\left. \begin{aligned} G_{\sigma_1 \sigma_2}^a(12) &= \frac{1}{i} \langle [\psi_{\sigma_1}(1), \psi_{\sigma_2}^\dagger(2)]_+ \rangle \eta_+(t_1 - t_2) \\ G_{\sigma_1 \sigma_2}^r(12) &= -\frac{1}{i} \langle [\psi_{\sigma_1}(1), \psi_{\sigma_2}^\dagger(2)]_+ \rangle \eta_+(t_2 - t_1) \end{aligned} \right\}$$

$\eta_+(t) = 1$ for $t > 0$ and 0 for $t < 0$. These are related to the causal Green's function defined above in a very simple way, being equal to the proper analytic continuation of $G_{\sigma_1 \sigma_2}(r_1 r_2; z)$ in their respective domains of definition.

To simplify the notation of Green's functions $G_{\sigma_1 \sigma_2}(12)$ may be written in the form of a matrix

$$G(12) = \begin{pmatrix} G_{\uparrow \uparrow}(12) & G_{\uparrow \downarrow}(12) \\ G_{\downarrow \uparrow}(12) & G_{\downarrow \downarrow}(12) \end{pmatrix} \quad (2.1.19)$$

This form resembles that used by Nambu [43] in his formulation of the superconductivity theory in which the off-diagonal Green's functions are the anomalous Green's functions. Let $(\tau_0, \tau_1, \tau_2, \tau_3)$ be the unit and the three Pauli matrices

$$\tau_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2.1.20)$$

Then the total number of particles is by definition $n(1) = \langle \psi^\dagger(1) \psi(1) + \psi^\dagger(1) \psi(1) \rangle$.

In view of (2.1.7, 8)

$$n(1) = -i [\text{tr } \tau_0 G(11^\dagger)] \quad (2.1.21a)$$

Similarly, the total spin moment is

$$\underline{\sigma}(1) = -i [\text{tr } \underline{\tau} G(11^\dagger)] \quad (2.1.21b)$$

with

$$\sigma_1(1) = -i [\text{tr } \tau_1 G(11^\dagger)] = \langle \psi^\dagger(1) \psi(1) + \psi^\dagger(1) \psi(1) \rangle \text{ etc.}$$

Here tr denotes the trace on the spin indices. The spin magnetic moment is given by $\frac{1}{2} \underline{\sigma} \mu_B$, where μ_B is the Bohr magneton.

The equation of motion satisfied by $G(11')$ (henceforth, no special symbol will indicate matrices are being used, unless otherwise stated) can now be constructed, since the Heisenberg equation for $\psi_{\sigma_1}(1)$ is

$$i \frac{\partial}{\partial t_1} \psi_{\sigma_1}(1) = \left[-\frac{\nabla_1^2}{2m} + V(1) \right] \psi_{\sigma_1}(1) + \sum_{\sigma_3} \int d^4\bar{3} \mathcal{U}(1-\bar{3}) \psi_{\sigma_3}^\dagger(\bar{3}) \psi_{\sigma_3}(\bar{3}) \psi_{\sigma_1}(1)$$

Here, in the third term on the right-hand side, the times of $\bar{3}$ and 1 are the same. Then,

$$\left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - V(1) \right] G_{\sigma_1 \sigma_2}(12) - \sum_{\sigma_3} \int d^4\bar{3} \mathcal{U}(1-\bar{3}) \frac{1}{i} \langle T(\psi_{\sigma_3}^\dagger(\bar{3}) \psi_{\sigma_3}(\bar{3}) \psi_{\sigma_1}(1) \psi_{\sigma_2}^\dagger(2)) \rangle = \delta_{\sigma_1 \sigma_2} \delta^{(4)}(1-2)$$

$\delta^{(4)}(1-2) = \delta^{(3)}(\underline{r}_1 - \underline{r}_2) \cdot \delta(t_1 - t_2)$. The last term in the left-hand side of this equation can be recast in terms of G and its variational derivative which will be defined presently. (For details refer KB Chapter 5). An extra source term

$$H' = \sum_{\sigma} \int d^3r U_{\sigma}(rt) \psi_{\sigma}^{\dagger}(rt) \psi_{\sigma}(rt) \quad (2.1.22)$$

is added to the Hamiltonian H , and this is made to vanish at the end of all calculations. The operators are still kept in the Heisenberg representation and the traces are also taken over the grand canonical ensemble pertaining to the total Hamiltonian. We shall not go into the redefinitions of G in the presence of U and we shall not even indicate by any symbol that G is evaluated in the presence of U unless otherwise stated. In view of this, the following well-known relationship is obtained: (which may also be taken as a definition)

$$i \frac{\delta}{\delta U(2)} \langle X(1) \rangle = \langle T(\psi^{\dagger}(2) \psi(2) X(1)) \rangle - \langle \psi^{\dagger}(2) \psi(2) \rangle \langle X(1) \rangle \quad (2.1.23)$$

since U generates $\psi^{\dagger} \psi$. This follows directly by developing $\langle X(1) \rangle$ as a power series in U and examining the term which is linear in U . Now

$$\frac{1}{i} \sum_{\sigma_3} \langle T(\psi_{\sigma_3}^{\dagger}(\bar{3}) \psi_{\sigma_3}(\bar{3}) \psi_{\sigma_1}(1) \psi_{\sigma_2}^{\dagger}(2)) \rangle$$

can be rewritten by using (2.1.23) as follows:

$$\sum_{\sigma_3} i \frac{\delta}{\delta U_{\sigma_3}(\bar{3}; t_3=t_1^+)} \langle T(\psi_{\sigma_1}(1) \psi_{\sigma_2}^\dagger(2)) \rangle$$

$$= \sum_{\sigma_3} \langle T(\psi_{\sigma_3}^\dagger(\bar{3}) \psi_{\sigma_3}(\bar{3}) \psi_{\sigma_1}(1) \psi_{\sigma_2}^\dagger(2)) \rangle - \sum_{\sigma_3} \langle \psi_{\sigma_3}^\dagger(\bar{3}) \psi_{\sigma_3}(\bar{3}) \rangle \langle T(\psi_{\sigma_1}(1) \psi_{\sigma_2}^\dagger(2)) \rangle$$

or equivalently

$$i \sum_{\sigma_3} \frac{\delta}{\delta U_{\sigma_3}(\bar{3}; t_3=t_1^+)} G(12) = \sum_{\sigma_3} \frac{1}{i} \langle T(\psi_{\sigma_3}^\dagger(\bar{3}) \psi_{\sigma_3}(\bar{3}) \psi_{\sigma_1}(1) \psi_{\sigma_2}^\dagger(2)) \rangle$$

$$+ [i \text{tr } \tau_0 G(\bar{3}\bar{3}^+)] G(12)$$

or

$$\frac{1}{i} \sum_{\sigma_3} \langle T(\psi_{\sigma_3}^\dagger(\bar{3}) \psi_{\sigma_3}(\bar{3}) \psi_{\sigma_1}(1) \psi_{\sigma_2}^\dagger(2)) \rangle$$

$$= i \sum_{\sigma_3} \frac{\delta G(12)}{\delta U_{\sigma_3}(\bar{3}; t_3=t_1^+)} - [i \text{tr } \tau_0 G(\bar{3}\bar{3}^+)] G(12)$$

Thus

$$\left\{ \left(i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - V(1) \right) \tau_0 + i \tau_0 \int d^4\bar{3} \mathcal{V}(1-\bar{3}) [\text{tr } \tau_0 G(\bar{3}\bar{3}^+)] \right\} G(12)$$

$$- \left[\left(\frac{1+\tau_3}{2} \right) U_\uparrow(1) + \left(\frac{1-\tau_3}{2} \right) U_\downarrow(1) \right] G(12) - i \sum_{\sigma_3} \int d^4\bar{3} \mathcal{V}(1-\bar{3}) \frac{\delta G(12)}{\delta U_{\sigma_3}(\bar{3}; t_3=t_1^+)}$$

$$= \tau_0 \delta^{(4)}(1-2).$$

We shall henceforth use $\tau_0 = 1$ or assume its presence. An inverse matrix Green's function may be formally introduced:

$$\left. \begin{aligned} \int G^{-1}(1\bar{2}) G(\bar{2}3) d^4\bar{2} &= \delta^{(4)}(1-3) \\ \int G(1\bar{2}) G^{-1}(\bar{2}3) d^4\bar{2} &= \delta^{(4)}(1-3) \end{aligned} \right\} \quad (2.1.24)$$

By taking the variational derivative of the second of these, and multiplying the resulting expression from the right by a suitable G , and using the first of the relations in (2.1.24) we obtain

$$\frac{\delta G(12)}{\delta U_{\sigma_3}(\bar{3})} = - \int d^4\bar{4} d^4\bar{5} G(1\bar{4}) \frac{\delta G^{-1}(\bar{4}\bar{5})}{\delta U_{\sigma_3}(\bar{3})} G(\bar{5}2) \quad (2.1.25)$$

We define a new function, $\Gamma_0(12; 3)$ which is often called the vertex part

$$\Gamma_0(12; 3) = \sum_{\sigma_3} \frac{\delta G^{-1}(12)}{\delta U_{\sigma_3}(\bar{3})} \quad (2.1.26)$$

Then

$$\left[i \frac{\partial}{\partial t_1} + \frac{V_1^2}{2m} - V(1) - \left(\frac{1+\tau_3}{2} \right) U_{\uparrow}(1) - \left(\frac{1-\tau_3}{2} \right) U_{\downarrow}(1) + i \int d^4\bar{3} \mathcal{V}(1-\bar{3}) [\text{tr} G(\bar{3}\bar{3}^+)] \right] G(12) \\ + i \int d^4\bar{3} d^4\bar{4} d^4\bar{5} \mathcal{V}(1-\bar{3}) G(1\bar{4}) \Gamma_0(\bar{4}\bar{5}; \bar{3}) G(\bar{5}2) = \delta^{(4)}(1-2) \quad (2.1.27)$$

Multiplying this on the right by $G^{-1}(21')$ and integrating over 2 and using (2.1.24) we get

$$\begin{aligned}
 G^{-1}(11') = & \left\{ i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - V(1) - \left(\frac{1+\tau_3}{2} \right) U_1(1) - \left(\frac{1-\tau_3}{2} \right) U_1(1) \right\} \delta^{(4)}(1-1') \\
 & + i \int d^4\bar{3} \mathcal{V}(1-\bar{3}) [\text{tr } G(\bar{3}\bar{3}^+)] \delta^{(4)}(1-1') \\
 & + i \int d^4\bar{3} d^4\bar{4} \mathcal{V}(1-\bar{3}) G(1\bar{4}) \Gamma_0(\bar{4}1'; \bar{3})
 \end{aligned} \tag{2.1.28}$$

The solution of this equation must obey the condition (2.1.10) when suitably extended into the imaginary time domain.

The new function Γ_0 may now be determined by writing an equation for it using its definition and the expression (2.1.28) for G^{-1} . This equation will now involve another new function $\delta\Gamma_0/\delta U$ and so on. Thus a chain of equations is obtained. The equation for Γ_0 is

$$\begin{aligned}
 \Gamma_0(12; 3) = & -\delta^{(4)}(1-2) \delta^{(4)}(1-3) - i \int d^4\bar{1} d^4\bar{2} d^4\bar{3} \mathcal{V}(1-\bar{1}) \text{tr} [G(\bar{1}\bar{2}) \Gamma_0(\bar{2}\bar{3}; 3) G(\bar{3}\bar{1}^+)] \\
 & \delta^{(4)}(1-2) \\
 & - i \int d^4\bar{1} d^4\bar{2} d^4\bar{3} d^4\bar{4} \mathcal{V}(1-\bar{1}) G(1\bar{3}) \Gamma_0(\bar{3}\bar{4}; 3) G(\bar{4}\bar{2}) \Gamma_0(\bar{2}2; \bar{1}) \\
 & + i \int d^4\bar{1} d^4\bar{2} \mathcal{V}(1-\bar{1}) G(1\bar{2}) \Gamma_{01}(\bar{2}2; \bar{1}3)
 \end{aligned} \tag{2.1.29}$$

where

$$\Gamma_{01}(\bar{2}2; \bar{1}3) = \sum_{\sigma_3} \frac{\delta}{\delta U_{\sigma_3}(3)} \Gamma_0(\bar{2}2; \bar{1}).$$

The various terms in (2.1.28) may be interpreted as follows. The last two terms are due to the two-particle interactions whereas the remaining terms arise from the single-particle parts in the Hamiltonian and the external source. The first of the last two terms is the Hartree self-energy, which, in the absence of external density disturbances, cancels precisely with the positive background. The last term contains the contributions from all kinds of scattering beginning with the exchange processes. (The Hartree term may also be thought of as arising from direct scattering processes). In view of this interpretation of the terms in G^{-1} , the terms on the right-hand side of (2.1.29) for Γ_0 may be similarly interpreted. The first term is due to the direct external perturbation, the second term arises from the density fluctuations stemming from the Hartree self energy, the third term includes all kinds of complicated scattering processes and the fourth contains various forms of corrections arising from changes in the vertices due to interactions. This last term is of second order in the interaction potential. The equation for Γ_0 is seen to be nonlinear and inhomogeneous. Because of this, as a crude first approximation, its solution may be taken to be just the inhomogeneous term. This, in (2.1.28) gives the well-known Hartree-Fock approximation.

Before discussing the various forms of these equations, a schematic outline of the method of solution of (2.1.28) will be given. Let $U_{\sigma} = 0$ in

(2.1.28) and the last two terms in it be denoted by

$$\begin{aligned} \sum (11') &= i \int d^4 T \mathcal{V}(1-\bar{T}) [\text{tr } G(\bar{T}T^+)] \delta^{(4)}(1-1') \\ &+ i \int d^4 T d^4 \bar{Z} \mathcal{V}(1-\bar{T}) G(1\bar{Z}) \Gamma_0(\bar{Z}1'; \bar{T}) . \end{aligned} \quad (2.1.30)$$

Here the Hartree energy is retained just for the sake of completeness. From its structure, it may be written in terms of $(1, \tau_1, \tau_2, \tau_3)$

$$\sum (11') = \alpha(11') + \underline{\tau} \cdot \underline{\beta}(11')$$

containing four unknown functions. When this is substituted back in (2.1.28),

$$G^{-1}(11') = \left(i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - V(1) \right) \delta^{(4)}(1-1') + \alpha(11') + \underline{\tau} \cdot \underline{\beta}(11') .$$

Hence G is expressed in terms of the unknown functions $\alpha, \underline{\beta}$. Putting this back in \sum , which contains G , fully determines the unknown functions.

So far no mention has been made of the geometric structure of the medium. Three cases will be considered. In the first two, the single-particle potential $V(r)$ will be taken to be identically zero, so that plane waves are the solutions for the noninteracting system. Here there are two possibilities. One is the translationally invariant case, while the second is the symmetry breaking solution of the Overhauser [18] type. In the third case $V(r)$ is taken to be a periodic potential such that the noninteracting system is now described by Bloch waves. Here again there are two cases

corresponding to the ones for the plane waves but only the symmetry preserving solutions will be here considered. (We need to know the nature of the non-interacting system, for the solutions of this are used as a complete set of states when the system is interacting in much the same way the normal modes of vibrations of a lattice are employed in treating the anharmonic vibrations).

2. Spatially Uniform Solutions

If the system is taken to be spatially uniform, then the Green's functions depend only on the space-time coordinate differences. In view of this one may take Fourier transforms in all the variables; the Fourier transform variable corresponding to the space coordinates has the significance of wave number for single particle states. Let, therefore,

$$G(p\omega) = \int d^4(l-l') e^{-ip \cdot (r_1 - r_{l'}) + i\omega(t_1 - t_{l'})} G(l-l') \quad (2.2.1)$$

We will often make use of the four-dimensional notation: $p \cdot l = (p \cdot r_1 - p_0 t_1)$; $p = (p, p_0)$, p_0 is a frequency or energy variable (which will be equivalently referred to as ω). Single G is a 2×2 matrix, it can be written in terms of unit and Pauli matrices:

$$G(l-l') = \frac{1}{2} [g(l-l') + \underline{\tau} \cdot \underline{\sigma}(l-l')] \quad (2.2.2)$$

Correspondingly, $g(p\omega)$ and $\underline{\sigma}(p\omega)$ are defined similarly to (2.2.1). Taking $t_{l'} = t_1 - 0$, we have from (2.1.6)

$$G(l-l')^+ = \frac{1}{2} [g(l-l')^+ + \underline{\tau} \cdot \underline{\sigma}(l-l')^+] = -iG^<(ll').$$

With this in (2.2.1) we may define (c.f. equations (2.1.21a, b))

$$n(\underline{p}) = \int \frac{d\omega}{2\pi i} g(\underline{p}, \omega) e^{i\omega o^+} = \text{total number of particles of momentum } \underline{p} \quad (2.2.3)$$

$$\underline{g}(\underline{p}) = \int \frac{d\omega}{2\pi i} \underline{g}(\underline{p}, \omega) e^{i\omega o^+} = \text{spin density of momentum } \underline{p}$$

The simplest approximation is to take the first term in (2.1.29) as the solution for Γ_o

$$\Gamma_o(12; 3) = -\delta^{(4)}(1-2) \delta^{(4)}(1-3) \quad (2.2.4)$$

The expression (2.1.28) for G^{-1} after taking $U = 0$ (also $V(r) = 0$ in the present calculation) takes the well-known Hartree-Fock form: (here the Hartree self-energy term is dropped as it is cancelled by the positive background)

$$G_{HF}^{-1}(1-1') = \left(i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} \right) \delta^{(4)}(1-1') - i \mathcal{V}(1-1') G_{HF}(1-1') \quad (2.2.5)$$

Taking Fourier transforms,

$$\begin{aligned} G_{HF}^{-1}(\underline{p}, \omega) &= \omega - \underline{p}^2/2m - i \int \frac{d^3 \underline{p}}{(2\pi)^4} \frac{d\bar{\omega}}{} \mathcal{V}(\underline{p} - \underline{\bar{p}}) G_{HF}^<(\underline{\bar{p}}, \bar{\omega}) e^{i\bar{\omega} o^+} \\ &= \omega - \underline{p}^2/2m - i \int \frac{d^3 \underline{p}}{(2\pi)^4} \frac{d\bar{\omega}}{} \mathcal{V}(\underline{p} - \underline{\bar{p}}) n_F(\bar{\omega}) A_{HF}(\underline{\bar{p}}, \bar{\omega}) e^{i\bar{\omega} o^+} \quad (2.2.6) \end{aligned}$$

as also by definition (2.2.3)

$$= \omega - \underline{p}^2/2m + \frac{1}{2} \int \frac{d^3 \underline{p}}{(2\pi)^3} \mathcal{V}(\underline{p} - \underline{\bar{p}}) (n(\underline{p}) + \underline{\tau} \cdot \underline{\sigma}(\underline{\bar{p}})). \quad (2.2.7)$$

From this G_{HF} can be obtained by inverting the right-hand side. Let

$$\begin{aligned} \omega_{\pm}(\underline{p}) &= \underline{p}^2/2m - \frac{1}{2} \int \mathcal{V}(\underline{p} - \underline{\bar{p}}) n(\underline{\bar{p}}) \frac{d^3 \underline{\bar{p}}}{(2\pi)^3} \\ &\mp \frac{1}{2} \left| \int \mathcal{V}(\underline{p} - \underline{\bar{p}}) \underline{\sigma}(\underline{\bar{p}}) \frac{d^3 \underline{\bar{p}}}{(2\pi)^3} \right| \end{aligned} \quad (2.2.8)$$

$$\begin{aligned} g_{\pm}(\underline{p}, \omega) &= 1/[\omega - \omega_{\pm}(\underline{p})] \\ \text{and} \quad \underline{\hat{s}}(\underline{p}) &= \text{unit vector of} \\ &\frac{1}{2} \int \mathcal{V}(\underline{p} - \underline{\bar{p}}) \underline{\sigma}(\underline{\bar{p}}) \frac{d^3 \underline{\bar{p}}}{(2\pi)^3} \end{aligned} \quad (2.2.9)$$

Then after reducing to partial fractions

$$\begin{aligned} G_{HF}(\underline{p}, \omega) &= \frac{1}{2} [g_{+}(\underline{p}, \omega) + g_{-}(\underline{p}, \omega)] \\ &+ \frac{1}{2} \underline{\tau} \cdot \underline{\hat{s}}(\underline{p}) [g_{+}(\underline{p}, \omega) - g_{-}(\underline{p}, \omega)] \end{aligned} \quad (2.2.10)$$

It is seen that in this approximation, there are two poles in the single-particle Green's function corresponding to the two spin orientations of the particles. If the last term is omitted, the usual HF states are recovered. Hence,

$$\left. \begin{aligned} g(\underline{p}, \omega) &= [g_+(\underline{p}, \omega) + g_-(\underline{p}, \omega)] \\ \underline{\sigma}(\underline{p}, \omega) &= \hat{g}(\underline{p}) [g_+(\underline{p}, \omega) - g_-(\underline{p}, \omega)] \end{aligned} \right\} \quad (2.2.3')$$

On integration over the ω plane as specified by (2.2.3) the following expressions are obtained:

$$\left. \begin{aligned} n(\underline{p}) &= [n_F(\omega_+(\underline{p})) + n_F(\omega_-(\underline{p}))] \\ \underline{\sigma}(\underline{p}) &= \hat{g}(\underline{p}) [n_F(\omega_+(\underline{p})) - n_F(\omega_-(\underline{p}))] \end{aligned} \right\} \quad (2.2.11)$$

with $n_F(x) =$ Fermi function. The above results were derived by Suris [17] also. Thus, defining $n(\underline{p})$ and $\underline{\sigma}(\underline{p})$ as in (2.2.3) and recalculating them in the HF approximation gives us the equations (2.2.11) to determine them. Note that ω_{\pm} contain $(n, \underline{\sigma})$. These equations are thus nonlinear integral equations for $n, \underline{\sigma}$ of the Hammerstein type. Suris (loc. cit.) used the theory of these equations to derive the usual Stoner results.

Discussion of a few aspects of these results may be in order here.

The up and down spin states are pushed apart and the energy difference is

$$\int \mathcal{V}(\underline{p} - \underline{\bar{p}}) \underline{\sigma}(\underline{\bar{p}}) d^3 \underline{\bar{p}} / (2\pi)^3.$$

This is proportional to the total magnetization if one assumed $\mathcal{V}(\underline{p}) = \overline{\mathcal{V}}$, independent of \underline{p} , or \mathcal{V} to be short ranged, since $\int \underline{\sigma}(\underline{p}) d^3 \underline{p} / (2\pi)^3$ is the total magnetization of the system. From (2.2.11) then, one has

$$|\underline{s}_{\text{total}}| = \int \frac{d^3 \underline{p}}{(2\pi)^3} \left[n_F(\underline{p}^2/2m - \frac{1}{2} \bar{v} N - \frac{1}{2} \bar{v} |\underline{s}_{\text{total}}|) \right. \\ \left. - n_F(\underline{p}^2/2m - \frac{1}{2} \bar{v} N + \frac{1}{2} \bar{v} |\underline{s}_{\text{total}}|) \right] \quad (2.2.12a)$$

and

$$N = \int \frac{d^3 \underline{p}}{(2\pi)^3} \left[n_F(\underline{p}^2/2m - \frac{1}{2} \bar{v} N - \frac{1}{2} \bar{v} |\underline{s}_{\text{total}}|) \right. \\ \left. + n_F(\underline{p}^2/2m - \frac{1}{2} \bar{v} N + \frac{1}{2} \bar{v} |\underline{s}_{\text{total}}|) \right] \quad (2.2.12b)$$

These are precisely the expressions assumed by Stoner[4] in his collective electron theory of ferromagnetism. Thus in the case of zero-range interaction, and in the HF approximation, Stoner's assumptions are fully justified. The Stoner's constant $K\theta'$ is seen to be related to \bar{v} through the relationship

$$\bar{v} = (2K\theta'/N) . \quad (2.2.13)$$

These results were derived by Suris [17] and also anticipated to some extent by Thompson [24]. They were included here for the sake of completeness and to provide a frame-work for generalization to the Bloch case and to the symmetry breaking solutions of the SDW type. Before deriving the Overhauser equations with the present formalism, the relations (2.2.3') will be recast in a form that corresponds to the Overhauser equations in the special case that the symmetry breaking parameter Q becomes zero. To see this, let us define

$$\underline{s}(\underline{p}) = \frac{1}{2} \int \underline{v}(\underline{p}-\underline{q}) \underline{\sigma}(\underline{q}) d^3 \underline{q} / (2\pi)^3 \quad (2.2.14)$$

(this is actually related to Overhauser's $g(\underline{p})$). Multiplying the second of (2.2.11) by $\mathcal{V}(\underline{p}-\underline{q})$ and integrating with respect to \underline{p} , we arrive at

$$\underline{s}(\underline{p}) = \frac{1}{2} \int \mathcal{V}(\underline{p}-\underline{q}) [n_F(\omega_+(\underline{q})) - n_F(\omega_-(\underline{q}))] \frac{\underline{s}(\underline{q})}{|\underline{s}(\underline{q})|} \frac{d^3 \underline{q}}{(2\pi)^3}.$$

But from (2.2.8)

$$|\omega_+(\underline{q}) - \omega_-(\underline{q})| = 2|\underline{s}(\underline{q})|.$$

Thus

$$\underline{s}(\underline{p}) = \int \mathcal{V}(\underline{p}-\underline{q}) \left[\frac{n_F(\omega_+(\underline{q})) - n_F(\omega_-(\underline{q}))}{\omega_+(\underline{q}) - \omega_-(\underline{q})} \right] \underline{s}(\underline{q}) \frac{d^3 \underline{q}}{(2\pi)^3} \quad (2.2.15)$$

3. Symmetry Breaking Solutions of the Overhauser Type

Besides the usual plane wave solutions of the HF equations, Overhauser [18] pointed out that there are symmetry breaking solutions which are also possible ground states of the system. Overhauser associates a plane wave of the form $\exp(i\mathbf{k} \cdot \mathbf{r})$ with the up spin and $\exp(i(\mathbf{k} + \mathbf{Q}) \cdot \mathbf{r})$ with the down spin. Thus the vector \mathbf{Q} is a measure of the inhomogeneity, or in other words, a measure of the breaking of translational symmetry. The unrestricted HF solutions of this type are alternative candidates for the ground state of the system equally acceptable as the conventional ones. Overhauser first introduces such a term into the HF equations and then finds conditions for consistency very similar in structure to (2.2.15). His $g(\mathbf{k})$ is seen to be a convolution of the interaction potential with the intrinsic spin density. To derive Overhauser's expressions, the following

redefinitions of the Fourier transforms of the Green's functions are necessary:

$$\left. \begin{aligned} G_{\uparrow\uparrow}(11') &= \int \frac{d^3 \underline{k}'}{(2\pi)^3} e^{i \underline{k}' \cdot (\underline{r}_1 - \underline{r}_{1'})} G_{\uparrow\uparrow}(\underline{k}'; t_1 - t_{1'}) \\ G_{\uparrow\downarrow}(11') &= \int \frac{d^3 \underline{k}'}{(2\pi)^3} e^{i (\underline{k}' + \underline{Q}) \cdot (\underline{r}_1 - \underline{r}_{1'})} G_{\uparrow\downarrow}(\underline{k}'; t_1 - t_{1'}) \\ G_{\downarrow\uparrow}(11') &= \int \frac{d^3 \underline{k}'}{(2\pi)^3} e^{i \underline{k}' \cdot \underline{r}_1 - i (\underline{k}' + \underline{Q}) \cdot \underline{r}_{1'}} G_{\downarrow\uparrow}(\underline{k}'; t_1 - t_{1'}) \\ G_{\downarrow\downarrow}(11') &= \int \frac{d^3 \underline{k}'}{(2\pi)^3} e^{i (\underline{k}' + \underline{Q}) \cdot \underline{r}_1 - i \underline{k}' \cdot \underline{r}_{1'}} G_{\downarrow\downarrow}(\underline{k}'; t_1 - t_{1'}) \end{aligned} \right\} \quad (2.3.1)$$

Then the HF equation (2.2.5) takes the form

$$G^{-1}(\underline{k}) = \begin{pmatrix} \omega - \epsilon_{\uparrow}(\underline{k}) & -g_{\uparrow\downarrow}(\underline{k}) \\ -g_{\downarrow\uparrow}(\underline{k}) & \omega - \epsilon_{\downarrow}(\underline{k} + \underline{Q}) \end{pmatrix} \quad (2.3.2)$$

where

$$\left. \begin{aligned} \epsilon_{\uparrow}(\underline{k}) &= \underline{k}^2/2m + i \int \mathcal{V}(\underline{k} - \underline{k}') G_{\uparrow\uparrow}^<(\underline{k}' \omega') e^{i\omega' o^+} \frac{d^3 \underline{k}' d\omega'}{(2\pi)^4} \\ \epsilon_{\downarrow}(\underline{k} + \underline{Q}) &= (\underline{k} + \underline{Q})^2/2m + i \int \mathcal{V}(\underline{k} - \underline{k}') G_{\downarrow\downarrow}^<(\underline{k}' \omega') e^{i\omega' o^+} \frac{d^3 \underline{k}' d\omega'}{(2\pi)^4} \\ g_{\uparrow\downarrow}(\underline{k}) &= i \int \mathcal{V}(\underline{k} - \underline{k}') G_{\uparrow\downarrow}^<(\underline{k}' \omega') e^{i\omega' o^+} \frac{d^3 \underline{k}' d\omega'}{(2\pi)^4} \\ g_{\downarrow\uparrow}(\underline{k}) &= i \int \mathcal{V}(\underline{k} - \underline{k}') G_{\downarrow\uparrow}^<(\underline{k}' \omega') e^{i\omega' o^+} \frac{d^3 \underline{k}' d\omega'}{(2\pi)^4} \end{aligned} \right\} \quad (2.3.3)$$

Hence, inverting we obtain

$$G(\underline{k}, \omega) = \frac{\begin{pmatrix} \omega - \epsilon_{\downarrow}(\underline{k} + \underline{Q}) & g_{\uparrow\downarrow}(\underline{k}) \\ g_{\uparrow\downarrow}(\underline{k}) & \omega - \epsilon_{\uparrow}(\underline{k}) \end{pmatrix}}{(\omega - \omega_{+}(\underline{k}))(\omega - \omega_{-}(\underline{k}))} \quad (2.3.4)$$

where

$$\omega_{\pm}(\underline{k}) = \left(\frac{\epsilon_{\uparrow}(\underline{k}) + \epsilon_{\downarrow}(\underline{k} + \underline{Q})}{2} \right) \pm \sqrt{\left(\frac{\epsilon_{\uparrow}(\underline{k}) - \epsilon_{\downarrow}(\underline{k} + \underline{Q})}{2} \right)^2 + g_{\uparrow\downarrow}(\underline{k}) g_{\uparrow\downarrow}(\underline{k})} \quad (2.3.5)$$

These are precisely the modified single-particle states due to the up-down coupling derived by Overhauser (loc. cit.). We may recast (2.3.4) in the following form to complete the connection with Overhauser's notation.

Putting the expressions (2.3.4) into partial fractions one obtains

$$G(\underline{k}, \omega) = \left\{ \begin{aligned} & \left\{ \frac{\omega_+(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})}{\omega_+(\underline{k}) - \omega_-(\underline{k})} g_+(\underline{k}, \omega) - \frac{\omega_-(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})}{\omega_+(\underline{k}) - \omega_-(\underline{k})} g_-(\underline{k}, \omega) \right\} \\ & \left\{ \frac{g_{f+}(\underline{k})}{\omega_+(\underline{k}) - \omega_-(\underline{k})} [g_+(\underline{k}, \omega) - g_-(\underline{k}, \omega)] \right\} \\ & \left\{ \frac{\omega_+(\underline{k}) - \epsilon_f(\underline{k})}{\omega_+(\underline{k}) - \omega_-(\underline{k})} g_+(\underline{k}, \omega) - \frac{\omega_-(\underline{k}) - \epsilon_f(\underline{k})}{\omega_+(\underline{k}) - \omega_-(\underline{k})} g_-(\underline{k}, \omega) \right\} \\ & \left\{ \frac{g_{f+}(\underline{k})}{\omega_+(\underline{k}) - \omega_-(\underline{k})} [g_+(\underline{k}, \omega) - g_-(\underline{k}, \omega)] - \frac{\omega_-(\underline{k}) - \epsilon_f(\underline{k})}{\omega_+(\underline{k}) - \omega_-(\underline{k})} g_-(\underline{k}, \omega) \right\} \end{aligned} \right\} \quad (2.3.6)$$

where

$$g_{\pm}(\underline{k}, \omega) = [1/(\omega - \omega_{\pm}(\underline{k}))]. \quad (2.3.6')$$

From (2.3.5) one has the following easily verifiable relationships

$$\begin{aligned} (\omega_+(\underline{k}) - \epsilon_f(\underline{k})) &= \left[- \left(\frac{\epsilon_f(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})}{2} \right) - \sqrt{\left(\frac{\epsilon_f(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})}{2} \right)^2 + g_{f+}(\underline{k}) g_{f-}(\underline{k})} \right] \\ &= -(\omega_-(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})) \end{aligned} \quad (2.3.7a)$$

$$\begin{aligned} (\omega_+(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})) &= \left[+ \left(\frac{\epsilon_f(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})}{2} \right) - \sqrt{\left(\frac{\epsilon_f(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})}{2} \right)^2 + g_{f+}(\underline{k}) g_{f-}(\underline{k})} \right] \\ &= -(\omega_-(\underline{k}) - \epsilon_f(\underline{k})) \end{aligned} \quad (2.3.7b)$$

$$(\omega_+(\underline{k}) - \omega_-(\underline{k})) = -2 \sqrt{\left(\frac{\epsilon_f(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})}{2} \right)^2 + g_{\uparrow\downarrow}(\underline{k}) g_{\downarrow\uparrow}(\underline{k})} \quad (2.3.7c)$$

$$(\omega_+(\underline{k}) - \epsilon_f(\underline{k})) (\omega_+(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})) = g_{\uparrow\downarrow}(\underline{k}) g_{\downarrow\uparrow}(\underline{k}) \quad (2.3.7d)$$

$$\left. \begin{aligned} (\omega_+(\underline{k}) - \epsilon_f(\underline{k}))^2 + g_{\uparrow\downarrow}(\underline{k}) g_{\downarrow\uparrow}(\underline{k}) &= \\ &= (\omega_+(\underline{k}) - \omega_-(\underline{k})) (\omega_+(\underline{k}) - \epsilon_f(\underline{k})) \\ (\omega_-(\underline{k}) - \epsilon_f(\underline{k}))^2 + g_{\uparrow\downarrow}(\underline{k}) g_{\downarrow\uparrow}(\underline{k}) &= \\ &= (\omega_+(\underline{k}) - \omega_-(\underline{k})) (\omega_-(\underline{k}) - \epsilon_f(\underline{k})) \end{aligned} \right\} \quad (2.3.7e)$$

as also

$$\left. \begin{aligned} (\omega_+(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q}))^2 + g_{\uparrow\downarrow}(\underline{k}) g_{\downarrow\uparrow}(\underline{k}) &= (\omega_+(\underline{k}) - \omega_-(\underline{k})) (\omega_+(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})) \\ (\omega_-(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q}))^2 + g_{\uparrow\downarrow}(\underline{k}) g_{\downarrow\uparrow}(\underline{k}) &= (\omega_+(\underline{k}) - \omega_-(\underline{k})) (\omega_-(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})) \end{aligned} \right\} \quad (2.3.7f)$$

From the coefficients of $g_+(\underline{k}\omega)$ and $g_-(\underline{k}\omega)$ in (2.3.6) it is reasonable to set

$$\left. \begin{aligned} \cos^2 \theta_{\underline{k}} &= \left[\frac{\omega_+(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})}{\omega_+(\underline{k}) - \omega_-(\underline{k})} \right] \\ \sin^2 \theta_{\underline{k}} &= - \left[\frac{\omega_-(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})}{\omega_+(\underline{k}) - \omega_-(\underline{k})} \right] \end{aligned} \right\} \quad (2.3.8)$$

whose sum is clearly unity.

From (2.3.7e, f) the choice of the branches ω_{\pm} may be removed and (2.3.7e, f) may be written as

$$\left. \begin{aligned} (\omega - \epsilon_f(\underline{k}))^2 + g_{f\downarrow}(\underline{k}) g_{f\uparrow}(\underline{k}) &= (\omega_+(\underline{k}) - \omega_-(\underline{k})) (\omega - \epsilon_f(\underline{k})) \\ (\omega - \epsilon_f(\underline{k} + \underline{Q}))^2 + g_{f\downarrow}(\underline{k}) g_{f\uparrow}(\underline{k}) &= (\omega_+(\underline{k}) - \omega_-(\underline{k})) (\omega - \epsilon_f(\underline{k} + \underline{Q})) \end{aligned} \right\} (2.3.7g)$$

Using these results for $(\omega_+(\underline{k}) - \omega_-(\underline{k}))$ in (2.3.8),

$$\cos^2 \theta_{\underline{k}} = \frac{(\omega_+(\underline{k}) - \epsilon_f(\underline{k} + \underline{Q})) (\omega_+(\underline{k}) - \epsilon_f(\underline{k}))}{(\omega_+(\underline{k}) - \epsilon_f(\underline{k}))^2 + g_{f\downarrow}(\underline{k}) g_{f\uparrow}(\underline{k})}$$

and in view of (2.3.7d)

$$\cos^2 \theta_{\underline{k}} = \frac{g_{f\downarrow}(\underline{k}) g_{f\uparrow}(\underline{k})}{(\omega_+(\underline{k}) - \epsilon_f(\underline{k}))^2 + g_{f\downarrow}(\underline{k}) g_{f\uparrow}(\underline{k})}$$

We could define quite generally

$$\cos^2 \theta_{\underline{k}} = \frac{g_{f\downarrow}(\underline{k}) g_{f\uparrow}(\underline{k})}{(\omega - \epsilon_f(\underline{k}))^2 + g_{f\downarrow}(\underline{k}) g_{f\uparrow}(\underline{k})} \quad (2.3.9)$$

with the specification of the branch and the definitions of $\theta_{\underline{k}}$ the same as given by Overhauser. Moreover, from (2.3.8) and (2.3.7d)

$$\begin{aligned}
 \cos^2 \theta_{\underline{k}} \sin^2 \theta_{\underline{k}} &= \frac{g_{\uparrow \downarrow}(\underline{k}) g_{\downarrow \uparrow}(\underline{k})}{(\omega_{+}(\underline{k}) - \omega_{-}(\underline{k}))^2} \\
 &= \frac{g_{\uparrow \downarrow}(\underline{k}) g_{\downarrow \uparrow}(\underline{k})}{4 \left[\left(\frac{\epsilon_{\uparrow}(\underline{k}) - \epsilon_{\downarrow}(\underline{k} + \underline{Q})}{2} \right)^2 + g_{\uparrow \downarrow}(\underline{k}) g_{\downarrow \uparrow}(\underline{k}) \right]} \quad (2.3.10)
 \end{aligned}$$

We may now write $G(\underline{k}\omega)$ as

$$G(\underline{k}\omega) = \begin{pmatrix} [\cos^2 \theta_{\underline{k}} g_{+}(\underline{k}\omega) + \sin^2 \theta_{\underline{k}} g_{-}(\underline{k}\omega)] \cos \theta_{\underline{k}} \sin \theta_{\underline{k}} \sqrt{\frac{g_{\uparrow \downarrow}(\underline{k})}{g_{\downarrow \uparrow}(\underline{k})}} (g_{+}(\underline{k}\omega) - g_{-}(\underline{k}\omega)) \\ \cos \theta_{\underline{k}} \sin \theta_{\underline{k}} \sqrt{\frac{g_{\downarrow \uparrow}(\underline{k})}{g_{\uparrow \downarrow}(\underline{k})}} (g_{+}(\underline{k}\omega) - g_{-}(\underline{k}\omega)) [\sin^2 \theta_{\underline{k}} g_{+}(\underline{k}\omega) + \cos^2 \theta_{\underline{k}} g_{-}(\underline{k}\omega)] \end{pmatrix} \quad (2.3.11)$$

These may be substituted back in (2.3.3) to give

$$\begin{aligned}
 \epsilon_{\uparrow}(\underline{k}) &= \underline{k}^2/2m - \int \frac{d^3 \underline{k}'}{(2\pi)^3} \mathcal{V}(\underline{k}-\underline{k}') [\cos^2 \theta_{\underline{k}, n_F(\omega_+(\underline{k}'))} + \sin^2 \theta_{\underline{k}, n_F(\omega_-(\underline{k}'))}] \\
 \epsilon_{\downarrow}(\underline{k} + \underline{Q}) &= \frac{(\underline{k} + \underline{Q})^2}{2m} - \int \frac{d^3 \underline{k}'}{(2\pi)^3} \mathcal{V}(\underline{k}-\underline{k}') [\sin^2 \theta_{\underline{k}, n_F(\omega_+(\underline{k}'))} + \cos^2 \theta_{\underline{k}, n_F(\omega_-(\underline{k}'))}] \\
 g_{\uparrow\uparrow}(\underline{k}) &= \int \frac{d^3 \underline{k}'}{(2\pi)^3} \mathcal{V}(\underline{k}-\underline{k}') \sqrt{\frac{g_{\uparrow\uparrow}(\underline{k}')}{g_{\uparrow\uparrow}(\underline{k})}} \cos \theta_{\underline{k}, \sin \theta_{\underline{k}, [n_F(\omega_+(\underline{k}')) - n_F(\omega_-(\underline{k}'))]} \\
 g_{\uparrow\downarrow}(\underline{k}) &= \int \frac{d^3 \underline{k}'}{(2\pi)^3} \mathcal{V}(\underline{k}-\underline{k}') \sqrt{\frac{g_{\uparrow\downarrow}(\underline{k}')}{g_{\uparrow\downarrow}(\underline{k})}} \cos \theta_{\underline{k}, \sin \theta_{\underline{k}, [n_F(\omega_+(\underline{k}')) - n_F(\omega_-(\underline{k}'))]}
 \end{aligned}
 \tag{2.3.12}$$

where the consistent sign of the square root in (2.3.10) must be used. If in these we take, as was done by Overhauser, $g_{\uparrow\uparrow} = g_{\uparrow\downarrow} = g$, and assume only $\omega_+(\underline{k}')$ is occupied, then we recover all of Overhauser's results including the definitions of $\cos \theta_{\underline{k}}$. Thus a generalization of the Overhauser results is here achieved. Moreover, if we take $\underline{Q} = 0$, we see immediately that

$$\omega_{\pm}(\underline{k}) = \frac{\underline{k}^2}{2m} - \frac{1}{2} \int \frac{d^3 \underline{k}'}{(2\pi)^3} \mathcal{V}(\underline{k}-\underline{k}') n(\underline{k}') \mp |\underline{s}(\underline{k})|$$

with $\underline{s}(\underline{k})$ defined as in (2.2.14), which are the same as those in (2.2.8). Also from (2.3.10)

$$\cos^2 \theta_{\underline{k}} \sin^2 \theta_{\underline{k}} = \frac{g_{\uparrow\downarrow}(\underline{k}) g_{\downarrow\uparrow}(\underline{k})}{4 |\underline{s}(\underline{k})|^2}$$

or

$$\cos \theta_{\underline{k}} \sin \theta_{\underline{k}} = \frac{\sqrt{g_{\uparrow\downarrow}(\underline{k}) g_{\downarrow\uparrow}(\underline{k})}}{2 |\underline{s}(\underline{k})|}$$

so that

$$\begin{aligned}
 g_{\frac{1}{2}}(\underline{k}) &= - \int \frac{d^3 \underline{k}'}{(2\pi)^3} \mathcal{V}(\underline{k}-\underline{k}') \frac{g_{\frac{1}{2}}(\underline{k}')}{2|\underline{s}(\underline{k}')|} (n_F(\omega_+(\underline{k}') - n_F(\omega_-(\underline{k}')))) \\
 &= \int \frac{d^3 \underline{k}'}{(2\pi)^3} \mathcal{V}(\underline{k}-\underline{k}') \frac{g_{\frac{1}{2}}(\underline{k}')}{(\omega_+(\underline{k}') - \omega_-(\underline{k}'))} (n_F(\omega_+(\underline{k}') - n_F(\omega_-(\underline{k}'))))
 \end{aligned}$$

which is the τ_1 component of the equation (2.2.15), etc. Thus, the Overhauser results are the generalizations of the usual Stoner conditions written in a slightly different form. Incidentally, (2.3.12) generalizes the Overhauser results for finite temperatures as well as for finite magnetization.

4. Homogeneous Solutions Involving Bloch Electrons

Here a brief description of the extension of the above results in the conventional case ($\underline{Q} = 0$) will be given for Bloch electrons. Let $b_{lk}(1)$ be the stationary Bloch function satisfying the Schrödinger equation

$$(-\nabla^2/2m + V(1))b_{lk}(1) = \epsilon_l(k) b_{lk}(1) \quad (2.4.1)$$

where l is the band index and k , the reduced wave vector of the electron. The Green's function in the Bloch k space can now be constructed (a continuum of k is here used for convenience) thus

$$G(11') = \sum_l \int_{\text{IBZ}} b_{lk}(1) b_{lk}^*(1') G(lk; t_1 - t_1') \frac{d^3 k}{(2\pi)^3} \quad (2.4.2)$$

Here IBZ implies that the sum on k is over those in the first Brillouin zone. This is now substituted in the HF equation (2.2.5), and neglecting

Umklapp processes, the Green's function in the HF scheme is derived; this is very similar to the plane wave case (2.2.10) but with the poles at

$$\omega_{l'}^{\pm}(p) = \epsilon_{l'}(p) - \frac{1}{2} \sum_{l''} \int \frac{d^3 q}{(2\pi)^3} \mathcal{V}(p-q) |\langle l_p | l'' q \rangle|^2 n_{l''}(q)$$

$$\mp \frac{1}{2} \left| \sum_{l''} \int \frac{d^3 q}{(2\pi)^3} \mathcal{V}(p-q) |\langle l_p | l'' q \rangle|^2 \underline{s}_{l''}(q) \right| \quad (2.4.3)$$

Here

$$\left. \begin{aligned} \mathcal{V}(\underline{k}) &= \int_{\text{unit cell}} e^{i \underline{k} \cdot \underline{r}} \mathcal{V}(|\underline{r}|) d^3 \underline{r}; \\ \langle l_p | l' q \rangle &= \int_{\text{unit cell}} u_{l_p}^*(\underline{r}) u_{l' q}(\underline{r}) d^3 \underline{r} \end{aligned} \right\} \quad (2.4.4)$$

where $u_{l_p}(\underline{r})$ is the periodic part of the Bloch function, $b_{l_p}(\underline{r})$. The self-consistency conditions (2.2.15) now take the form

$$\underline{s}_{l'}(p) = \sum_{l''} \int \frac{d^3 q}{(2\pi)^3} \mathcal{V}(p-q) |\langle l_p | l'' q \rangle|^2 \cdot$$

$$\cdot \left[\frac{n_F(\omega_{l'}^+(q)) - n_F(\omega_{l'}^-(q))}{|\omega_{l'}^+(q) - \omega_{l'}^-(q)|} \right] \underline{s}_{l'}(q) \quad (2.4.5)$$

This represents a system of equations in which the band polarizations are coupled. The neglect of Umklapp processes is justified if the bands are broad and the local field corrections neglected (Adler [44]). It must also

be pointed out that in deriving (2.4.3) one neglects the contributions from other determinantal states (or, the configuration interactions are neglected). These appear in the present formalism since the second quantization technique includes all the determinants that can be constructed out of $b_{fk}(1)$. The properties of the Bloch functions are such that the matrix elements of the two-particle interaction potential has a restriction only on its k vector parts and not on the band indices. This implies that there are contributions to the matrix elements from all the four band indices and only three wave vectors.

5. Discussion of the Ground-State Properties

In the last few sections the single-particle Green's functions for a polarized interacting electron gas are studied in the HF scheme. This shows that the single-particle states in HF split into two, corresponding to the two directions of quantization of the electrons, parallel and antiparallel to the internal polarization. In the present section, the ground-state energy of the system is computed using the Green's functions derived so far. It can be shown that the expectation value of the Hamiltonian (2.1.1) with $U = 0$, can be written as

$$\begin{aligned} \frac{\langle H \rangle}{\Omega_0} &= \frac{-i}{4\Omega_0} \lim_{t \rightarrow t_1, +0} \int \text{tr} \left\{ \left[i \frac{\partial}{\partial t_1} - i \frac{\partial}{\partial t_{1'}} \right] + \right. \\ &\quad \left. + \left(-\frac{\nabla_1^2}{2m} - \frac{\nabla_{1'}^2}{2m} \right) G(11') \right\} d^3 r_1 \quad (\Omega_0: \text{ volume of the system}) \end{aligned} \quad (2.5.1)$$

This is related to the free energy, F , of the system through the relationship

$$-\frac{\partial}{\partial \beta} (\beta F) = \langle H \rangle / \Omega_0. \quad (2.5.2)$$

It is, however, the ground-state energy when $T = 0^\circ\text{K}$. We shall discuss the homogeneous and the Overhauser cases separately (the latter is included only for the sake of completeness).

(a) In the spatially uniform case, using the Fourier transforms as in (2.2.1) for $G(11')$, and performing the indicated operations in (2.5.1) one finally arrives at

$$\frac{\langle H \rangle}{\Omega_0} = \frac{1}{2} \int \text{tr} [(p_0 + p^2/2m) G(p, p_0)] e^{ip_0 0^+} \frac{d^3 p}{(2\pi)^3} \frac{dp_0}{2\pi i}. \quad (2.5.3)$$

Here we have used a four-dimensional notation as explained earlier. From (2.1.27) (with $U = 0$, $V = 0$) it is easy to verify after defining the Fourier transform of Γ_0 to be

$$\Gamma_0(12; 3) = \int \frac{d^4 p d^4 q}{(2\pi)^8} e^{ip(1-2) + iq(1-3)} \Gamma_0(p; q) \quad (2.5.4)$$

that

$$\begin{aligned} & [p_0 - p^2/2m + i\mathcal{V}(p=0) \int [\text{tr } G(p_2)] e^{ip_2 0^+} \frac{d^4 p_2}{(2\pi)^4} + \\ & + i \int \mathcal{V}(p-p_2) G(p_2) \Gamma_0(p; p-p_2) e^{ip_2 0^+} \frac{d^4 p_2}{(2\pi)^4}] G(p) = 1 \end{aligned} \quad (2.5.5)$$

Let us call the last two terms in brackets in the left side of (2. 5. 5), $\sum(p)$, which is a 2×2 matrix. Then formally one has

$$G(p) = \frac{1}{p_0 - p^2/2m + \sum(p p_0)}$$

Putting this in (2. 5. 3) and after some manipulation, one gets finally

$$\begin{aligned} \frac{\langle H \rangle}{\Omega_0} = & \frac{1}{i} \int \frac{d^4 p}{(2\pi)^4} \frac{p^2/2m}{p_0 - p^2/2m + \sum(p p_0)} [\text{tr } G(p)] e^{ip_0 0^+} - \\ & - \frac{1}{2} \mathcal{V}(p=0) \left(\int \frac{d^4 p}{(2\pi)^4} [\text{tr } G(p)] e^{ip_0 0^+} \right)^2 - \\ & - \frac{1}{2} \int \int \frac{d^4 p d^4 q}{(2\pi)^8} \mathcal{V}(p-q) [\text{tr } (G(q) \Gamma_0(p; p-q) G(p))] e^{ip_0 0^+} e^{iq_0 0^+} \end{aligned} \quad (2. 5. 6)$$

This is quite general and involves no approximations. The first term is the kinetic energy, the second is the Hartree energy and the third term contains energy due to all the interactions save the direct Hartree term. The appearance of Γ_0 in only the last term is significant. From this it follows, as will be shown soon, that the Hartree term will not be screened at all by the interactions. It is to show this, that the Hartree term was here retained. It drops out in the present problem, being cancelled by the positive background. The expression for the ground-state energy in the HF approximation is obtained by setting $\Gamma_0(p; q) = -1$. Then the above expression simplifies after using the HF Green's functions (2. 2. 10)

$$\begin{aligned}
\frac{\langle H \rangle_{HF}}{\Omega_0} = & \int \frac{d^3 q}{(2\pi)^3} \frac{q^2}{2m} [n_F(\omega_+(q)) + n_F(\omega_-(q))] - \\
& - \frac{1}{4} \int \int \frac{d^3 p d^3 q}{(2\pi)^6} \mathcal{V}(p-q) \left\{ [n_F(\omega_+(q)) + n_F(\omega_-(q))] [n_F(\omega_+(p)) + n_F(\omega_-(p))] + \right. \\
& \left. + \hat{z}(p) \cdot \hat{z}(q) [n_F(\omega_+(q)) - n_F(\omega_-(q))] [n_F(\omega_+(p)) - n_F(\omega_-(p))] \right\} \quad (2.5.7)
\end{aligned}$$

Suris [17] also derived an expression for the total energy in this form.

So far no restriction has been made on the form of the interaction potential, $\mathcal{V}(q)$. It will be shown in the next chapter that $\Gamma_0(p; p-q)$ is proportional to the inverse of a propagating dielectric constant. In the RPA, this dielectric function can be explicitly computed. In the static limit and for a long wavelength, this gives rise to a Thomas-Fermi screening. The same screening reappears when the collective excitations are studied. Thus, for the purpose of the present investigation we shall use a Yukawa interaction potential with arbitrary screening parameter, and study the nature of the solutions as a function of this screening (c.f. Robinson et.al., [37]).

We take the Yukawa potential in the form

$$\mathcal{V}(r) = e^2 (\exp - \xi k_F r) / r ,$$

where k_F is the paramagnetic Fermi momentum, ξ is a dimensionless parameter and e^2 is the square of the electronic charge. We also assume that

$$\left. \begin{aligned} n_F(\omega_+(q)) &= \eta_+(k_F - q) \\ n_F(\omega_-(q)) &= \eta_-(k_F - q) \end{aligned} \right\} \quad (2.5.8)$$

$k_{F\uparrow}$ and $k_{F\downarrow}$ are given by

$$\left. \begin{aligned} k_{F\uparrow} &= (1 + \zeta)^{1/3} k_F \\ k_{F\downarrow} &= (1 - \zeta)^{1/3} k_F \end{aligned} \right\} \quad (2.5.9)$$

where ζ is the relative magnetization and

$$(k_{F\uparrow}^3 + k_{F\downarrow}^3) / 6\pi^2 = N = \text{total number} = k_F^3 / 3\pi^2$$

η_+ is the positive unit step function. Furthermore, the G 's are assumed to be diagonal, equivalent to having the internal polarization in the z direction. The single-particle energies in the HF approximation then have the following form (c. f. (2.2.8)) at $T = 0^\circ K$:

$$\begin{aligned} \omega_{\pm}(p) &= \frac{p^2}{2m} - e^2/\pi p \left\{ p k_F (1 \pm \zeta)^{1/3} + \right. \\ &+ \left(\frac{p^2 - \xi^2 k_F^2 - (1 \pm \zeta)^{2/3} k_F^2}{4} \right) \ln \left| \frac{\xi^2 k_F^2 + (p - (1 \pm \zeta)^{1/3} k_F)^2}{\xi^2 k_F^2 + (p + (1 \pm \zeta)^{1/3} k_F)^2} \right| \\ &\left. - \xi k_F p \left(\tan^{-1} \left(\frac{p + (1 \pm \zeta)^{1/3} k_F}{\xi k_F} \right) - \tan^{-1} \left(\frac{p - (1 \pm \zeta)^{1/3} k_F}{\xi k_F} \right) \right) \right\} \end{aligned} \quad (2.5.10)$$

Evaluating $\langle H \rangle / \Omega_0$ under the same approximations, one has for the total energy per electron in the HF approximation

$$\mathcal{E}_{HF}(\zeta) = \langle H \rangle_{HF} / \Omega_0 N = \mathcal{E}_{\uparrow}(\zeta) + \mathcal{E}_{\downarrow}(\zeta) \quad (2.5.11)$$

with

$$\left. \begin{aligned} \mathcal{E}_1(\xi) &= \frac{3}{5} \frac{(1+\xi)^{5/3}}{2} \left(\frac{1}{ar_s}\right)^2 - \frac{3}{4\pi} \left(\frac{1}{ar_s}\right)(1+\xi)^{4/3} \mathcal{F}(\xi/2(1+\xi)^{1/3}) \\ \mathcal{E}_1(\xi) &= \frac{3}{5} \frac{(1-\xi)^{5/3}}{2} \left(\frac{1}{ar_s}\right)^2 - \frac{3}{4\pi} \left(\frac{1}{ar_s}\right)(1-\xi)^{4/3} \mathcal{F}(\xi/2(1-\xi)^{1/3}) \end{aligned} \right\} \quad (2.5.12)$$

where we have introduced $ar_s = me^2/k_F$, $a = (4/9\pi)^{1/3} = 0.521$, and

$$\mathcal{F}(z) = \left\{ 1 - \frac{2}{3} z^2 - \frac{8}{3} z \tan^{-1}(1/z) + \frac{2}{3} z^2 (z^2 + 3) \ln(1 + 1/z^2) \right\}. \quad (2.5.13)$$

$\mathcal{F}(z)$ has the following features. It is unity at $z = 0$ and monotonically decreases to zero as z increases, and for $z \gg 1$, $\mathcal{F}(z) \sim 1/9 z^2$, which is obtained by expanding $\mathcal{F}(z)$ in a power series of $1/z$. A schematic diagram of its behavior is given in Fig. 3.

The coupling strengths must be defined properly when the two extreme limits $\xi = 0$ and $\xi = \infty$ are considered. These are displayed in Table 3. From this table it is clear that one may infer the Coulomb behavior for $\xi \ll 1$ and the short-range behavior for $\xi \gg 1$. The precise value of ξ for which this transition takes place will be given later in this section. Also, the coupling strengths in the two limits are seen to be related through the last expression in the table. Let us redefine the energy per particle in terms of the Fermi energy so that we only need to examine a dimensionless quantity:

$$\begin{aligned} \mathcal{E}(\xi) = & \frac{3}{5} \left[\frac{(1+\xi)^{5/3} + (1-\xi)^{5/3}}{2} \right] - \\ & - \frac{9}{16} \left(\frac{K\theta'}{\epsilon_F} \right) \xi^2 \left[(1+\xi)^{4/3} \mathcal{J} \left(\frac{\xi}{2(1+\xi)^{1/3}} \right) + (1-\xi)^{4/3} \mathcal{J} \left(\frac{\xi}{2(1-\xi)^{1/3}} \right) \right] \end{aligned}$$

(2.5.14)

The absolute minimum of this as a function of the magnetization for various values of ξ will now be examined.

TABLE 3 The Yukawa Potential and the Various Limits

$$\mathcal{V}(r) = e^2 (\exp - \xi k_F r) / r ; \mathcal{V}(q) = 4\pi e^2 / (q^2 + \xi^2 k_F^2)$$

k_F : Fermi momentum.

For $\xi \ll 1$, $\mathcal{V}(q) = 4\pi e^2 / q^2$ Coulomb potential

We define the coupling strength as $g_C = \alpha r_s$

(r_s in Bohr units) ($\alpha = (4/9\pi)^{1/3} = 0.521$)

For $\xi \gg 1$, $\mathcal{V}(q) = 4\pi e^2 / \xi^2 k_F^2 = \text{a constant } \bar{\mathcal{V}}$

(Stoner) zero range potential

We define the coupling strength $g_s = m \bar{\mathcal{V}} k_F / 2\pi^2$

$$= (2\alpha r_s) / \pi \xi^2$$

In terms of the Stoner coupling strength from (2.2.13)

$$g_S = 3/2 (K\theta' / \epsilon_F) , \quad \epsilon_F = \text{Fermi energy } (\xi = 0)$$

Thus

$$K\theta' / \epsilon_F = 4/3 (\alpha r_s / \pi \xi^2) .$$

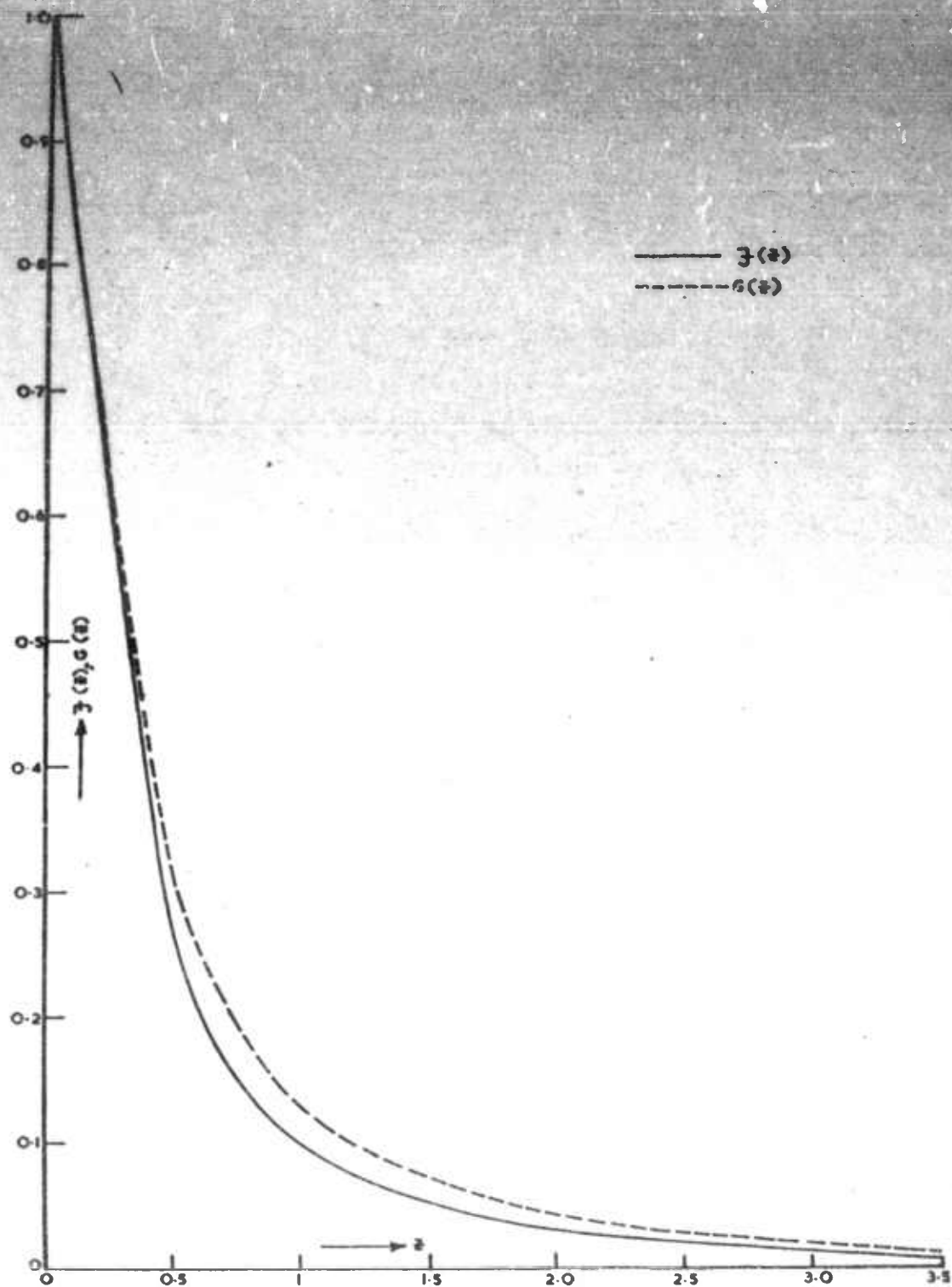


FIG. 3: PLOT OF $f(z)$ AND $g(z)$ VS z (SCHEMATIC)

As $\mathcal{E}(\xi)$ is defined on a closed interval, the end points must be discussed separately. For the interior points $0 < \xi < 1$ one has the usual derivative conditions:

$$\text{and } \left. \begin{aligned} \partial \mathcal{E} / \partial \xi &= 0 \\ \partial^2 \mathcal{E} / \partial \xi^2 &> 0 \end{aligned} \right\} \quad (0 < \xi < 1) \quad (2.5.15)$$

The first condition gives

$$\left(\frac{K\theta'}{\epsilon_F} \right)_{\min} = \frac{2}{3\xi^2} \left[\frac{(x^2 - y^2)}{x G(\xi/2x) - y G(\xi/2y)} \right] \quad (0 < \xi < 1) \quad (2.5.16)$$

where

$$G(z) = (1 - 2z \tan^{-1}(1/z) + z^2 \ln(1 + 1/z^2)). \quad (2.5.17)$$

$G(z)$, like $\mathcal{F}(z)$, is monotonically decreasing with increasing z , taking the value unity for $z = 0$, and going to zero like $1/6z^2$ for large z . A plot of this is given in Fig. 3. In the above $x = (1 + \xi)^{1/3}$ and $y = (1 - \xi)^{1/3}$. We have to examine the sign of $\partial^2 \mathcal{E} / \partial \xi^2$ which is given by (2.5.18) to ascertain the existence of a minimum in this interval:

$$\begin{aligned} \frac{\partial^2 \mathcal{E}}{\partial \xi^2} = \frac{\xi^2}{4} \left(\frac{K\theta'}{\epsilon_F} \right)_{\min} & \left\{ - \frac{(x-y)^2}{x^2 y^2} - \frac{2\xi}{xy(x-y)} \left(\tan^{-1} \left(\frac{2x}{\xi} \right) - \tan^{-1} \left(\frac{2y}{\xi} \right) \right) + \right. \\ & + \frac{\xi^2(x+y)}{4xy(x-y)} \left[\left(\frac{2x-y}{x} \right) \ln \left(\frac{\xi^2 + 4x^2}{\xi^2} \right) + \right. \\ & \left. \left. + \left(\frac{x-2y}{y} \right) \ln \left(\frac{\xi^2 + 4y^2}{\xi^2} \right) \right] \right\} \quad (2.5.18) \end{aligned}$$

Before discussing these in detail, a remark concerning (2.5.16) may be in order. It must be noted that the definitions (2.5.8) and (2.5.9) make the relations (2.2.11) a tautology. But if $k_{F\uparrow}$ and $k_{F\downarrow}$ are identified with the common chemical potential for the two spins by the relationship

$$\mu = \omega_+(k_{F\uparrow}) = \omega_-(k_{F\downarrow})$$

then (2.5.16) follows. Here ω_{\pm} are as in (2.5.10). This shows that the definitions (2.5.9) are consistent. This will be touched upon again later.

The following trivial lemma is of great use in deciding the sign of $\partial^2 \mathcal{E} / \partial \zeta^2$. Consider a function

$$\mathcal{E}(\zeta) = f(\zeta) - \text{ar}_s g(\zeta, \xi) \quad (0 \leq \zeta \leq 1). \quad (2.5.19a)$$

Then

$$\frac{\partial \mathcal{E}(\zeta)}{\partial \zeta} = 0 \quad \text{gives} \quad (\text{ar}_s)_{\min} = f'(\zeta) / g'(\zeta, \xi) \quad (0 < \zeta < 1) \quad (2.5.19b)$$

where primes denote differentiation. And

$$\begin{aligned} \frac{\partial^2 \mathcal{E}}{\partial \zeta^2} &= f''(\zeta) - (\text{ar}_s)_{\min} g''(\zeta, \xi) = g'(\zeta) \frac{d}{d\zeta} [f'(\zeta) / g'(\zeta, \xi)] \\ &= g'(\zeta) \left[\frac{d}{d\zeta} (\text{ar}_s)_{\min} \right] \quad (0 < \zeta < 1) \end{aligned} \quad (2.5.19c)$$

The sign of $\partial^2 \mathcal{E} / \partial \zeta^2$, therefore, depends on the variation of $(\text{ar}_s)_{\min}$ as a function of ζ provided $g'(\zeta, \xi)$ is shown to be positive throughout $0 < \zeta < 1$.

In view of this lemma, a plot of $(K\delta' / \epsilon_F)$ versus ζ for various ξ is given in Fig. 4. It is easy to show that $g'(\zeta, \xi)$, which corresponds

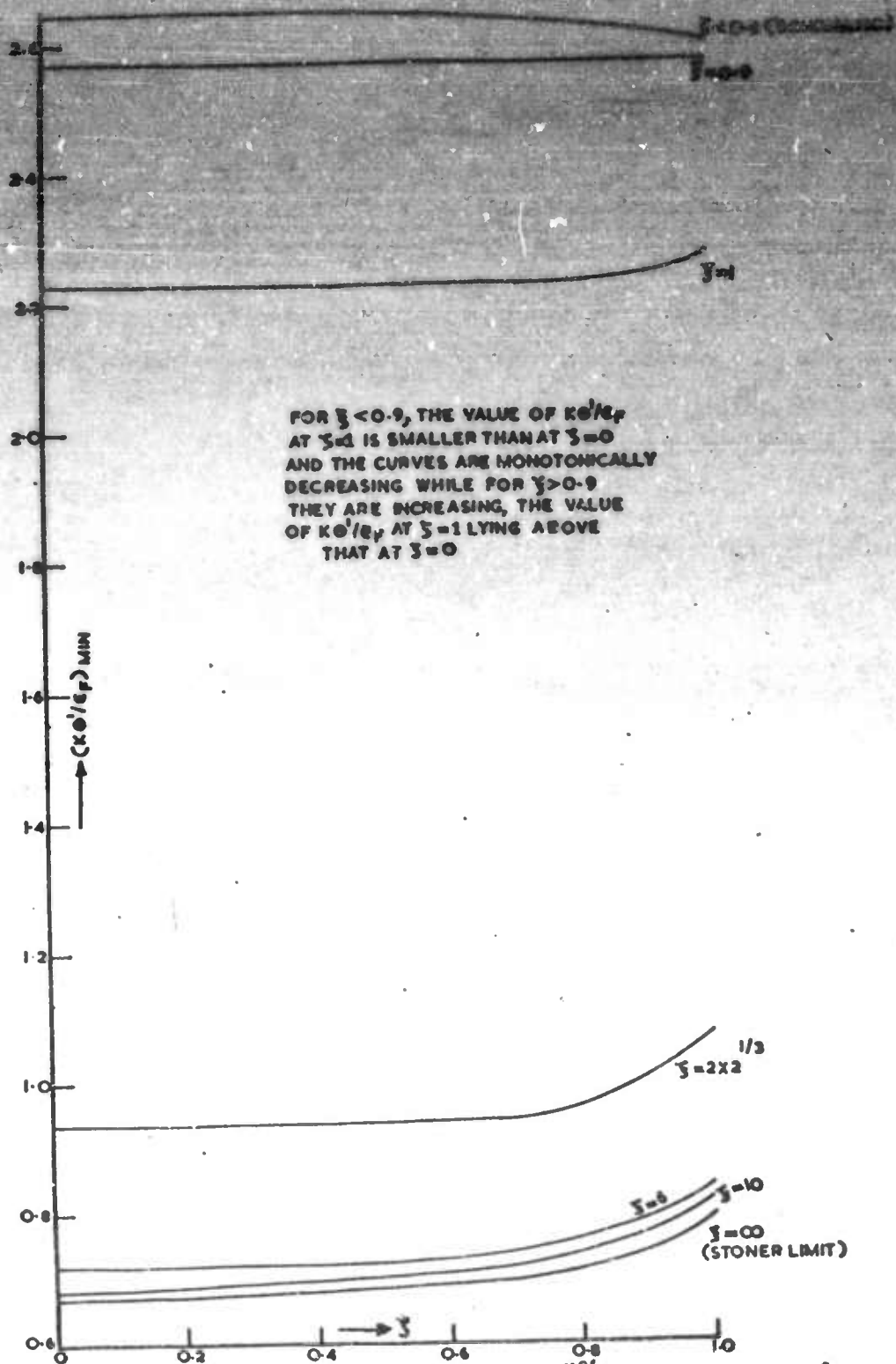


FIG. 4: PLOT OF $K\theta'/\epsilon_F$ VS. ξ THAT MAKES $\epsilon'(\xi, \xi, \frac{K\theta'}{\epsilon_F})$ VANISH FOR VARIOUS ϵ

to the derivative of the exchange energy with respect to ξ in $0 < \xi < 1$ is positive, by just examining it directly. The plots in Fig. 4 show that $(K\theta/\epsilon_F)_{\min}$ are monotonically increasing with ξ for $\xi \rightarrow \infty$ down to $\xi = 1$, and becoming monotonically decreasing for $\xi < 0.9$, the $\xi = 0.9$ curve being almost flat. This shows that for $0.9 < \xi < \infty$, $\partial^2 \mathcal{E} / \partial \xi^2 > 0$ for $0 < \xi < 1$ giving the possibility of a minimum in this range, while for $0 < \xi < 0.9$, $\partial^2 \mathcal{E} / \partial \xi^2 < 0$, and hence the intermediate states, $0 < \xi < 1$, are relative maxima and so are inadmissible as ground states. After this, one must compare the interior minimum with the values at the end points to arrive at the absolute minimum.

In the Coulomb and in the Stoner case, the following situations arise and are here given for the sake of completeness.

1. $\xi = 0$: Coulomb gas (Bloch [3])

From (2.5.14), since $\mathcal{F}(z=0) = 1$,

$$\begin{aligned} \mathcal{E}(\xi) = & \frac{3}{5} \left[\frac{(1+\xi)^{5/3} + (1-\xi)^{5/3}}{2} \right] - \\ & - \frac{3}{4\pi} \arcsin [(1+\xi)^{4/3} + (1-\xi)^{4/3}] \\ & (0 \leq \xi \leq 1) \end{aligned} \quad (2.5.20)$$

From (2.5.16)

$$(\arcsin)_{\min} = \frac{\pi}{2} [(1+\xi)^{1/3} + (1-\xi)^{1/3}] \quad (0 < \xi < 1) \quad (2.5.21)$$

$(\arcsin)_{\min}$ is a monotonically decreasing function of ξ , taking a value of about π near $\xi = 0$, and 0.63π near $\xi = 1$. Hence, the intermediate states

do not occur as ground states in the Coulomb case. More explicitly from (2.5.18),

$$(g^2 \mathcal{E} / g \zeta^2)_{(ar_s)_{\min}} = - (ar_s)_{\min} (x-y)^2 / 3x^2 y^2 < 0 \quad (0 < \zeta < 1) \quad (2.5.22)$$

So then one needs to compare just the energies of the P and the F states.

This gives the usual conditions of Bloch, namely, for $ar_s > 2.839$, one has F.

To see explicitly the equivalence of (2.5.21) with consistent definitions of $k_{F\uparrow}$ and $k_{F\downarrow}$, we have

$$\mu = k_{F\uparrow}^2 / 2m - \left(\frac{ar_s}{4}\right) k_F k_{F\uparrow} = k_{F\downarrow}^2 / 2m - \left(\frac{ar_s}{4}\right) k_F k_{F\downarrow}$$

from which the rest are obvious.

2. $\xi \sim \infty$: Stoner Gas (Stoner [4]; Suris [17])

From (2.5.14), since $\mathcal{F}(z) \sim 1/9 z^2$ for $z \rightarrow \infty$,

$$\mathcal{E}(\zeta) = \frac{3}{5} \left[\frac{(1+\zeta)^{5/3} + (1-\zeta)^{5/3}}{2} \right] - \frac{1}{2} \left(\frac{K\theta'}{\epsilon_F} \right) (1+\zeta^2) \quad (0 \leq \zeta \leq 1) \quad (2.5.23)$$

From (2.5.16), since $G(z) \sim 1/6 z^2$ for $z \rightarrow \infty$,

$$\left(\frac{K\theta'}{\epsilon_F} \right)_{\min} = \left[\frac{(1+\zeta)^{2/3} - (1-\zeta)^{2/3}}{2\zeta} \right] \quad (0 < \zeta < 1) \quad (2.5.24)$$

$(K\theta'/\epsilon_F)_{\min}$ is monotonically increasing with ζ , taking a value of about 0.67 near $\zeta = 0$ and about 0.79 near $\zeta = 1$, and, hence, the intermediate states can be ground states. More explicitly from (2.5.18),

$$(\partial^2 \mathcal{E} / \partial \xi^2) (K\theta' / \epsilon_F)_{\min} = \left(\frac{K\theta'}{\epsilon_F} \right)_{\min} \frac{(x-y)^2}{3xy} \quad (0 < \xi < 1) \quad (2.5.25)$$

This is positive and so the unsaturated ferromagnetic states can be ground states. From these one may infer the usual Stoner criteria.

The definition of chemical potential here is

$$\mu = k_{F\uparrow}^2 / 2m - \frac{1}{2} \overline{\mathcal{V}} N (1 + \xi) = k_{F\downarrow}^2 / 2m - \frac{1}{2} \overline{\mathcal{V}} N (1 - \xi)$$

from which the equivalence of (2.5.24) with consistent definitions of $k_{F\uparrow}$ and $k_{F\downarrow}$ follow.

3. Yukawa Case

The extreme cases of $\xi = 0$ and $\xi = \infty$ having been reviewed, the cases with finite ξ 's will now be discussed. First of all, the possibility of intermediate states will be discussed in view of the lemma quoted earlier (2.5.19c). In Fig. 4, a plot of $(K\theta' / \epsilon_F)_{\min}$ versus ξ for various values of ξ ranging from 0.5 to ∞ is given. From the expressions (2.5.14, 16, 18) one notices that the usual Taylor expansion for small arguments when ξ is large, indicates the Stoner-type behavior. This sort of argument gives the inequality that for $\xi \gg 2 \frac{1}{(1+\xi)^{1/3}}$ one obtains the short-range behavior and for $\xi \ll 2 \frac{1}{(1-\xi)^{1/3}}$ one obtains the long-range behavior. From Table 3, we had earlier obtained an estimate which is a factor $\frac{1}{2}$ of what is expected as above. More careful analysis shows that for $\xi \sim 0.9$ the transition from the "long-range" to the "short-range" behavior sets in, in the sense that the intermediate states tend to be disallowed for $\xi < 0.9$ and

allowed for $\xi > 0.9$. This is brought out clearly when Fig. 4 is examined in conjunction with the lemma.

In Figs. 5a-e a plot of $\mathcal{E}(\xi)$ versus ξ for various ξ but for several fixed $(K\theta'/\epsilon_F)$ are given. These plots show some interesting features. In Fig. 5a, $K\theta'/\epsilon_F = 0.2$ which in the Stoner limit exhibits the P state as ground state. It is seen that the P state is the absolute minimum for all ξ . In Fig. 5b, $K\theta'/\epsilon_F = 0.667$, which in the Stoner limit shows the absolute minimum precisely at $\xi = 0$. As ξ is decreased the curves look exactly as in Fig. 5a, showing that for finite ξ , P is still preferred. For $K\theta'/\epsilon_F = 0.68$, the Stoner curve shows a minimum at $\xi = 0.5$, i. e., UF is the ground state. This minimum moves to $\xi = 0$ quickly as ξ is decreased. This movement of the minima as ξ decreases is well brought out in Figs. 5d, e. In Fig. 5d, $K\theta'/\epsilon_F = 0.794$ where the Stoner limit gives the F state as the absolute minimum. On this plot, $\xi = 6$ is seen to exhibit an absolute minimum for some $\xi \neq 1$, and for $\xi = 2 \times 2^{1/3}$, P is the ground state, showing that as ξ decreases the absolute minimum ξ_{\min} moves to the left. In the last figure of this series, $K\theta'/\epsilon_F = 2$ where the Stoner curve is well in the F state. As ξ decreases, one gets UF for certain ξ , and for smaller ξ , the P state.

To show these more explicitly, a plot of $(K\theta'/\epsilon_F)$ versus ξ is given in Fig. 2b, such that this movement of the ξ_{\min} is brought out clearly. For a given $(K\theta'/\epsilon_F)$, as ξ is varied, we have the minima at various magnetizations. Conversely, for a given ξ_{\min} , there is a set of optimum values of $(K\theta'/\epsilon_F)$

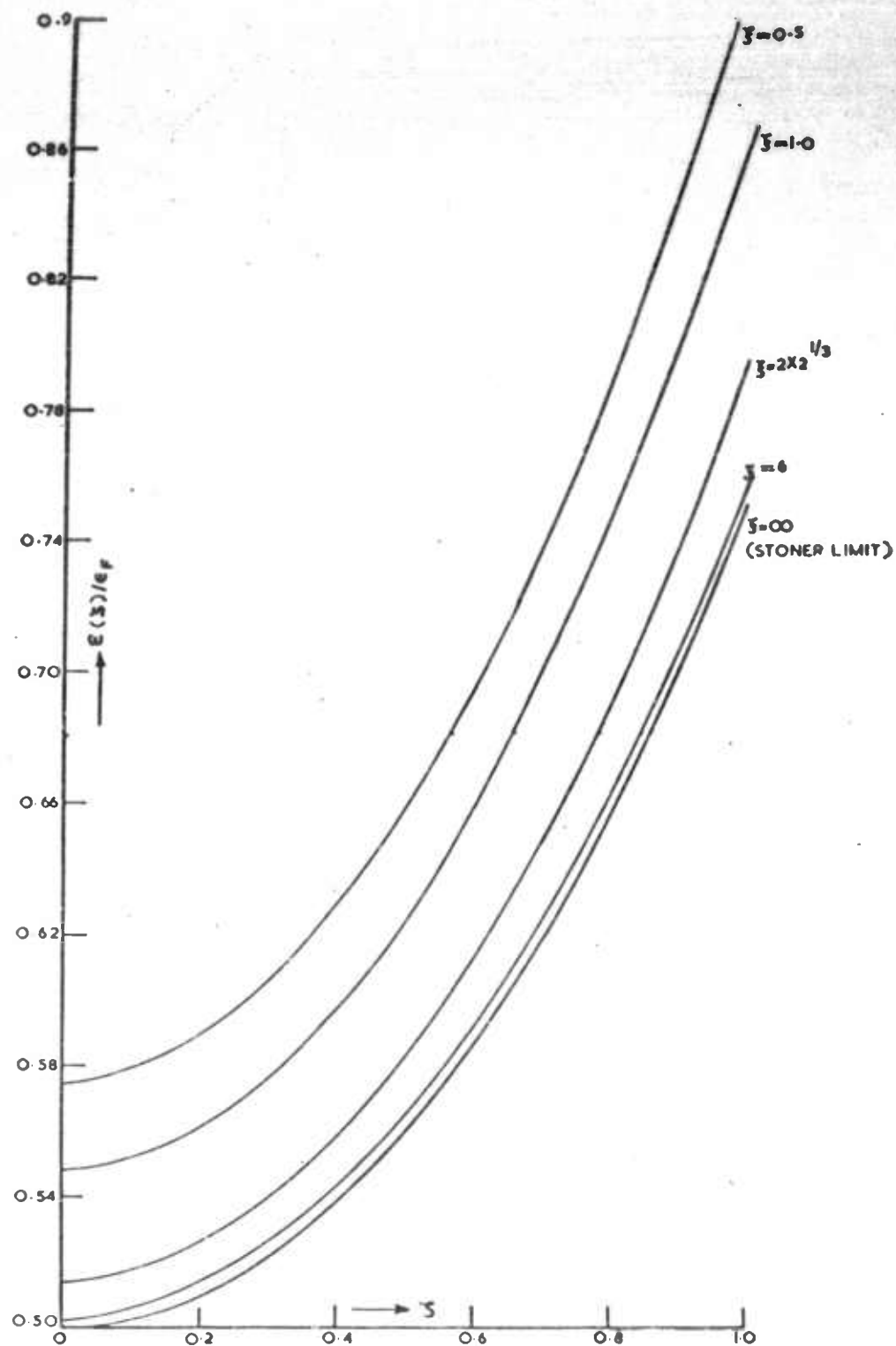


FIG. 5Q: $K\theta^1/\epsilon_F = 0.2$ FOR WHICH THE STONER CURVE IS FULLY PARAMAGNETIC.

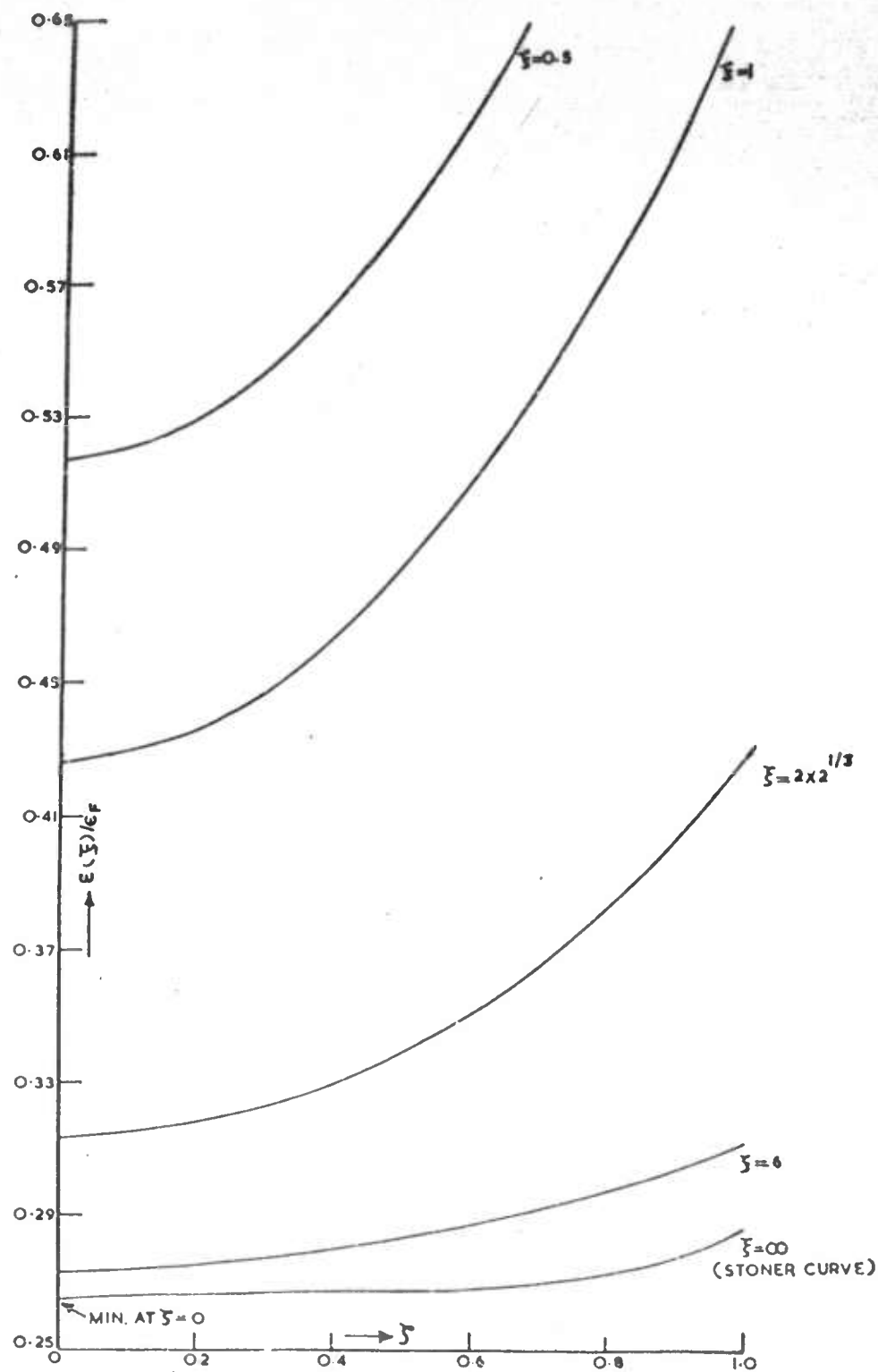


FIG. 5.b: $K\theta'/\epsilon_F=0.667$ FOR WHICH THE STONER CURVE HAS MINIMUM AT $\xi=0$

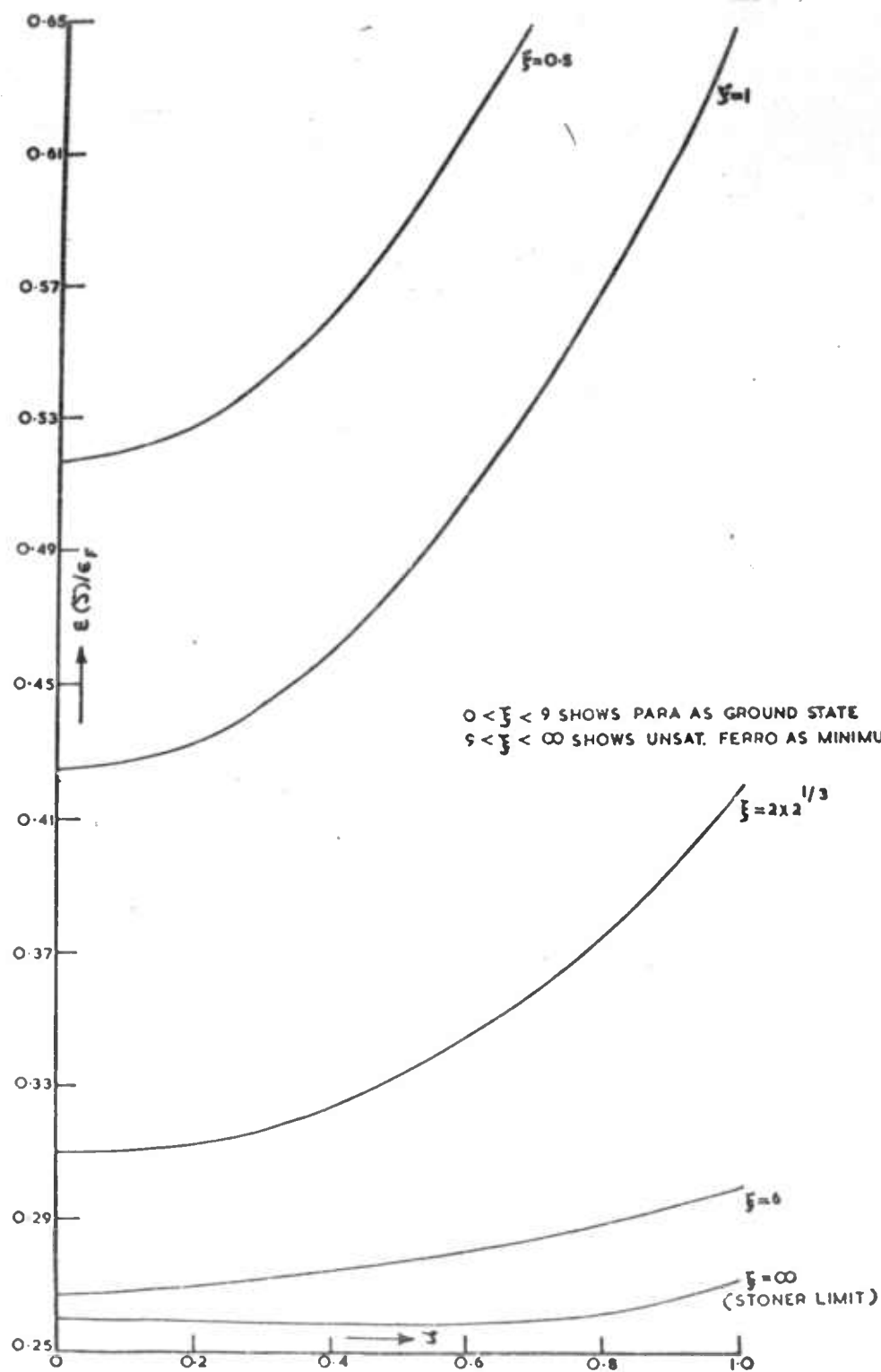


FIG. 5C: $K \theta^1/E_F = 0.68$ FOR WHICH THE STONER CURVE HAS A MINIMUM AT $S = 0.5$

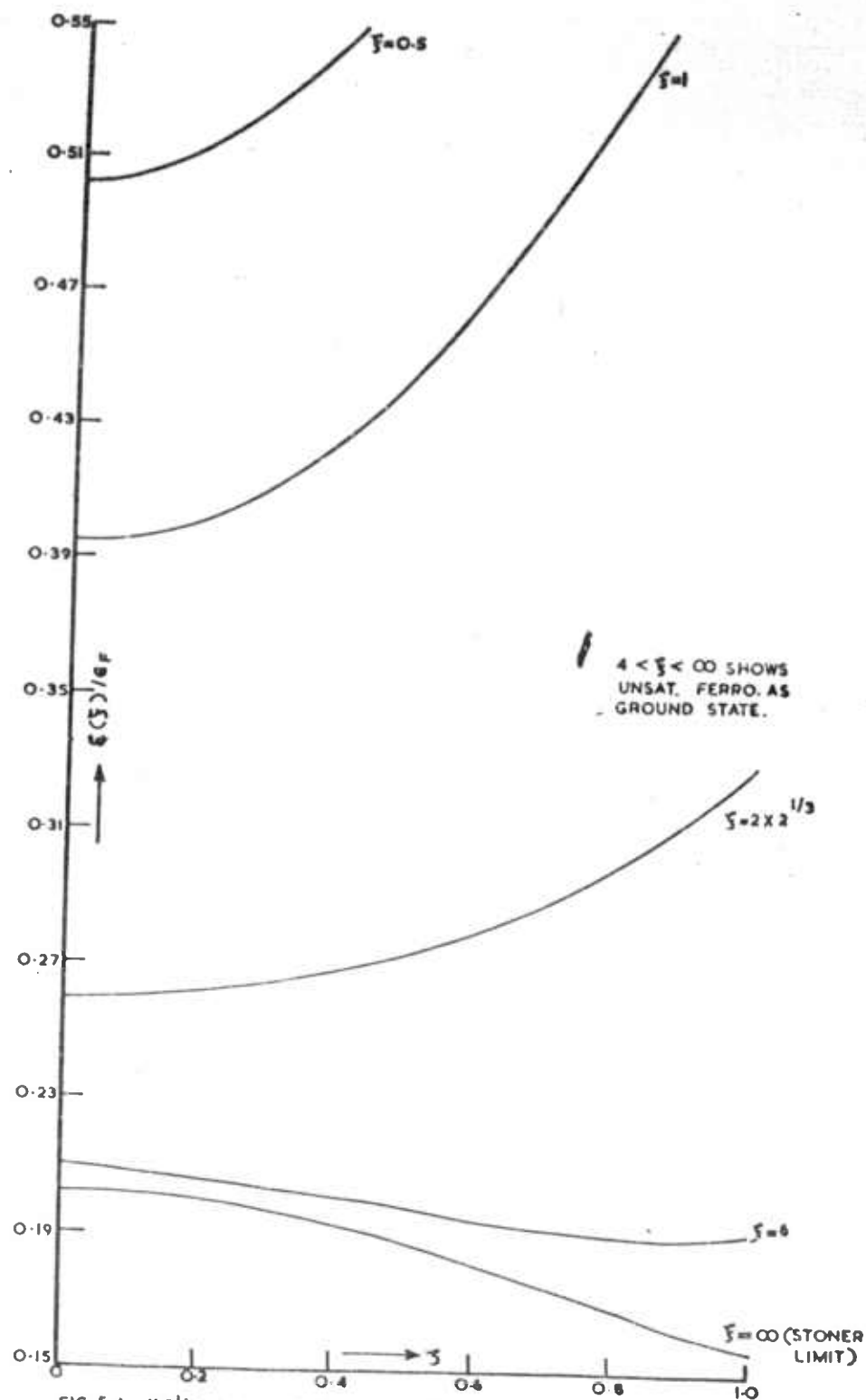


FIG. 5d: $K\theta'/\epsilon_F \approx 0.794$ FOR WHICH THE STONER CURVE HAS MINIMUM AT $\xi=1$

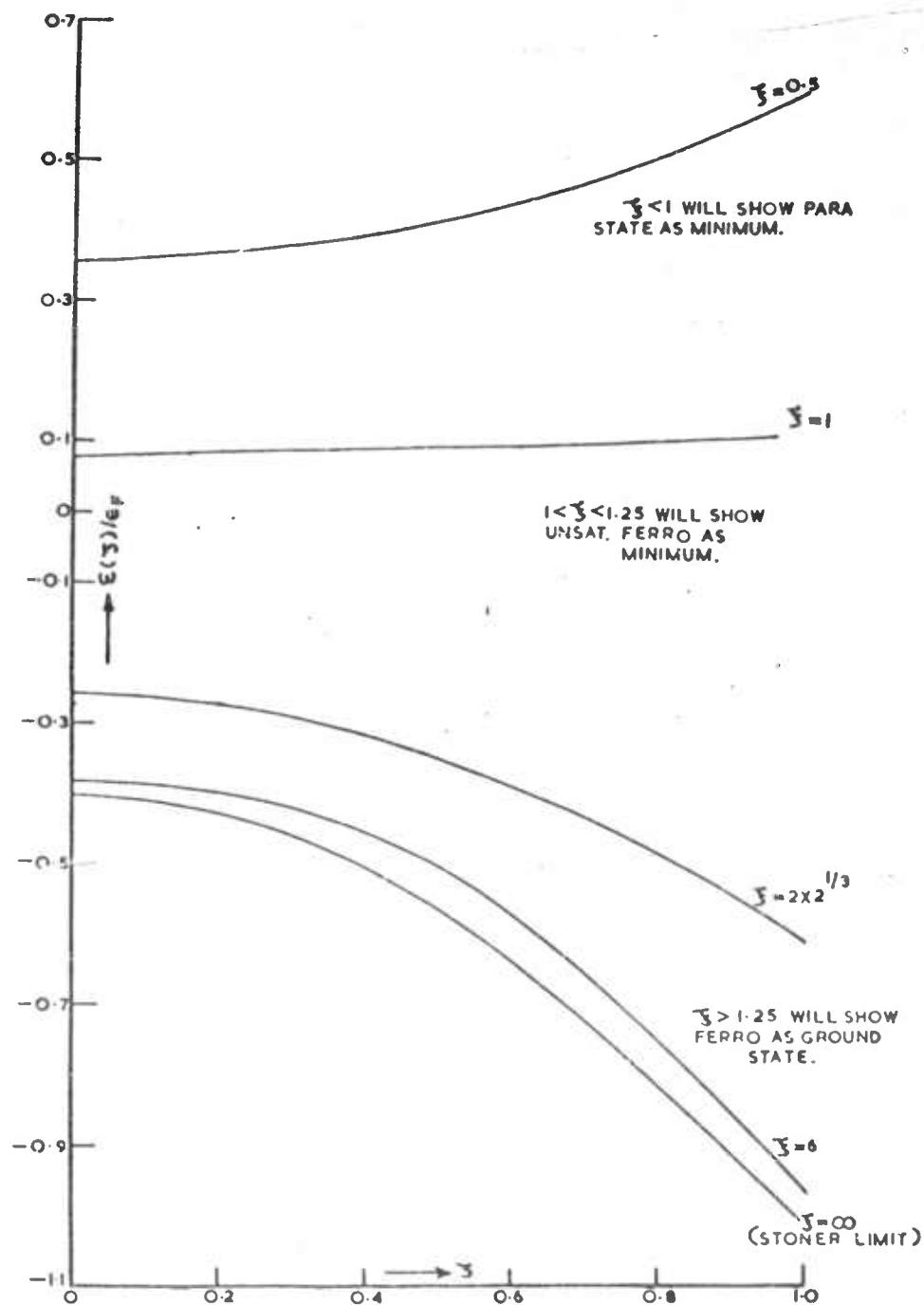


FIG. 5e: $k_0'/\epsilon_F = 2$ FOR WHICH THE STONER CURVE IS FULLY FERROMAGNETIC.

and ξ which minimize the total energy. This is obvious from Figs. 5a - e. For $\xi \rightarrow \infty$, above $K\theta'/\epsilon_F = 0.79$ one has F state and below $K\theta'/\epsilon_F = 0.67$ one has P state and between these two one has UF as ground states. As ξ is decreased, the region of UF becomes smaller and smaller, giving a higher and higher $(K\theta'/\epsilon_F)$ and finally at about $\xi = 0.9$, coalesce, showing that UF is no longer preferred below $\xi = 0.9$. Below this, one uses the condition obtained by just comparing the F and P states. For the sake of showing how the Bloch limit is obtained for $\xi = 0$, a similar plot of $\ln(ar_g)$ versus ξ is given in Fig. 2a. On this same figure, a plot of the Thomas-Fermi screening versus $\ln(ar_g)$ is also given. This plot never crosses the ferromagnetic region for any (ar_g) , showing that F state never occurs in HF for an electron gas with Thomas-Fermi screening.

(b) Just for the sake of completeness we derive the expression for $\langle H \rangle / \Omega_0$ in the Overhauser SDW case. From (2.5.1), using the Overhauser Green's functions (2.3.1) and (2.3.6) or evaluating $\langle H \rangle$ directly, we get

$$\begin{aligned}
\frac{\langle H \rangle}{\Omega_0} = & \int \frac{d^3 q}{(2\pi)^3} \left[\left(\frac{q^2}{2m} \cos^2 \theta_q + \frac{(q+Q)^2}{2m} \sin^2 \theta_q \right) n_F(\omega_+(q)) + \right. \\
& \left. + \left(\frac{q^2}{2m} \sin^2 \theta_q + \frac{(q+Q)^2}{2m} \cos^2 \theta_q \right) n_F(\omega_-(q)) \right] - \\
& - \frac{1}{2} \iint \frac{d^3 q d^3 q'}{(2\pi)^6} \mathcal{V}(q-q') \left\{ (\cos^2 \theta_q n_F(\omega_+(q)) + \right. \\
& + \sin^2 \theta_q n_F(\omega_-(q))) (\cos^2 \theta_{q'} n_F(\omega_+(q')) + \sin^2 \theta_{q'} n_F(\omega_-(q'))) + \\
& + (\sin^2 \theta_q n_F(\omega_+(q)) + \cos^2 \theta_q n_F(\omega_-(q))) (\sin^2 \theta_{q'} n_F(\omega_+(q')) + \cos^2 \theta_{q'} n_F(\omega_-(q'))) + \\
& + 2 \sqrt{\frac{g_{\uparrow\downarrow}(q) g_{\uparrow\downarrow}(q')}{g_{\uparrow\uparrow}(q) g_{\uparrow\uparrow}(q')}} \cos \theta_q \sin \theta_q \cos \theta_{q'} \sin \theta_{q'} (n_F(\omega_+(q)) - n_F(\omega_-(q))) \\
& \left. (n_F(\omega_+(q')) - n_F(\omega_-(q'))) \right\} \quad (2.5.26)
\end{aligned}$$

If, as Overhauser [18] did, only the $\omega_+(q)$ branch is assumed to be occupied and further $g_{\uparrow\downarrow} = g_{\uparrow\uparrow} = g$, we recover his expression. Incidentally, this generalizes Overhauser's results to finite temperatures. Treating θ_q as a variational parameter, one recovers back the condition on $\tan 2\theta_q$ which can be obtained from (2.3.8) also. Moreover, this generalizes Overhauser's results for intermediate magnetizations whereas Overhauser's work concerned only the paramagnetic state.

Summarizing, we have in this chapter discussed single particle states and the ground states of a polarized electron gas. The discussion

includes some formal results about SDW (symmetry breaking solutions) and electrons in a periodic potential (Bloch electrons). It is shown that the exchange energy in general is a very complicated function of g^2 , and not just a power series in g^2 . The main results are displayed in Figs. 2a, b which give the regions of magnetizations for optimum values of the coupling strengths and screening which minimize the total energy of the system. The use of the Thomas-Fermi screening is valid under certain approximations for a Coulomb gas, and implies a definite relationship between the screening and (ar_s) . From this it is shown that in HF the electron gas can never become ferromagnetic. All the calculations reported here are within the HF approximation and for zero temperature, though the formalism contains results for finite temperatures also.

III. INDIVIDUAL PARTICLE AND COLLECTIVE EXCITATION OF THE SYSTEM

1. General Introduction

In order to study the collective excitations of the system one needs to study the characteristic correlation functions. The formalism developed in the last chapter can be used for this purpose. In this section the necessary equations are derived for the correlation functions of interest. In view of the complications drastic approximations are made to solve them. These will be discussed in the next two sections.

The first-order response of a system to a given external perturbation can be expressed in terms of retarded correlation functions. There is a locus of poles in these functions in the frequency-momentum plane. This locus gives a relation between the frequency and the wave vector corresponding to the forcing field. These are the bound states or the collective states of the medium indicating resonant response to the external field. There is a second frequency-wave vector relationship which is not a pole structure in the correlation function but which is a branch singularity. The branch singularities correspond to the scattering states of the system. In general, the poles of the correlation function have a real and an imaginary part. The locus in the frequency-wave vector plane which makes this imaginary part non-zero gives a locus of a complex pole in this plane, showing that the collective part has a finite lifetime. When this imaginary part is zero one has a real pole which is the bound state excitation which occurs only for a certain range of the wave vector in a certain approximation. These may be stated physically as follows. In looking

for the collective excitations normally examined (and also those studied here), one looks for coherent motion of a particle-hole pair with certain characteristics, like their spin, wave vector and energy. The bound state corresponds to this coherent motion. Beyond a certain value of the wave vector (difference in the wave vectors of the pair) which is the wave vector of the collective mode, this coherence is lost and one no longer has a collective mode. This is the beginning of the scattering states of the system. Thus, the nature of the singularities in the retarded correlation functions tells us about the nature of the excitations in the medium. Here, in particular, the responses of the system to three kinds of external fields are studied: (1) oscillating fields giving rise to the fluctuations in the charge density of the medium thus yielding the density-density oscillations; these may also be thought of as a singlet state oscillation of the particle-hole pair; (2) oscillations of the z component of spin density by means of an external magnetic field in the z direction fluctuating the z component of spin density so as to create spin density oscillations without the attendant flipping of spin; these are the triplet oscillations of the pair with their projection zero; and (3) fields which fluctuate the transverse components of spin density by means of an external magnetic field in the other transverse direction giving rise to spin flip oscillations but without the fluctuations in the total charge density, thus leading to spin-wave type collective modes. These are the triplet state oscillations of the pair whose projection is unity. Instead of examining the retarded correlation functions themselves directly, a set of time-ordered

functions which are related to these (in the same way as in Chapter 2 concerning the single particle states) will be studied. This is done because the variational derivative technique can be used to advantage.

Define

$$\hat{\sigma}_i(1) = \sigma_i(1) - \langle \sigma_i \rangle \quad (i=0, 1, 2, 3) \quad (3.1.1)$$

where σ_i is the operator $\text{tr}(\psi^\dagger \tau_i \psi)$, ψ is taken to be a 1×2 column matrix, and $\langle \sigma_i \rangle$ is the usual average density as in (2.1.21a, b), where τ_i stands for the Pauli matrices and τ_0 for unit matrix. Thus, $\hat{\sigma}_0(1) = \text{excess particle density over the mean particle density, } \rho(1)$, $\hat{\sigma}_i(1) = \text{excess spin density over its mean}$. With these definitions the following correlation functions are computed:

$$\chi_{ij}(11') = \frac{1}{i} \langle T(\hat{\sigma}_i(1) \hat{\sigma}_j(1')) \rangle$$

$$(i, j = 0, +, -, 3) \quad (3.1.2)$$

The time ordering here corresponds to the Bose operators in contrast to Chapter II. For $i = j = 0$, ($\chi_{00} = \gamma_0$) this function is related to the dielectric constant, ϵ ; for $i = j = 3$, it is related to the longitudinal spin susceptibility, χ_{33} ; for $i = 1(+)$, $j = 2(-)$, it is related to the transverse susceptibility χ_{+-} . (1, 2 now refer to the spherical components $(\sigma_1 \pm i\sigma_2)/2$ instead of Cartesian components as in Chapter II).

As in Chapter II, Section 1, a set of formal relationships can be derived just on the basis of the definitions (3.1.2). These are given in Appendix A.

To relate the functions (3.1.2) to the variational derivatives with respect to external fields, let us first note that the fields U_{\uparrow} and U_{\downarrow} introduced in the last chapter may be combined to give the generators of total density and the z component of spin density by forming the following combinations:

$$U_{\uparrow} = U_0 + U_3 \quad \text{and} \quad U_{\downarrow} = U_0 - U_3 \quad (3.1.4)$$

so that (2.1.22) may now be written as

$$H' = \int d^3r [U_0(r) n(r) + U_3(r) \sigma_3(r)] \quad (3.1.5)$$

where

$$n(r) = \psi_{\uparrow}^{\dagger}(r) \psi_{\uparrow}(r) + \psi_{\downarrow}^{\dagger}(r) \psi_{\downarrow}(r)$$

and

$$\sigma_3(r) = \psi_{\uparrow}^{\dagger}(r) \psi_{\uparrow}(r) - \psi_{\downarrow}^{\dagger}(r) \psi_{\downarrow}(r)$$

In view of this we have

$$\frac{\delta}{\delta U_{\uparrow}} + \frac{\delta}{\delta U_{\downarrow}} = \frac{\delta}{\delta U_0}; \quad \frac{\delta}{\delta U_{\uparrow}} - \frac{\delta}{\delta U_{\downarrow}} = \frac{\delta}{\delta U_3}$$

To generate $\sigma_+(r) = \psi_{\uparrow}^{\dagger}(r) \psi_{\downarrow}(r)$

and

$$\sigma_-(r) = \psi_{\downarrow}^{\dagger}(r) \psi_{\uparrow}(r)$$

one introduces the following additional Hamiltonian

$$H'' = \int d^3r [U_+(r) \sigma_-(r) + U_-(r) \sigma_+(r)] \quad (3.1.6)$$

The fields (U_+, U_-, U_3) , when suitably chosen, are the components of a space- and time-dependent external magnetic field. The equation for the single particle

Green's function in the presence of all these fields may now be written down as in the last chapter (here no new notation is introduced to distinguish this from the old one as this does not cause any confusion) corresponding to (2.2.28)

$$\begin{aligned}
 G^{-1}(11') = & \left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - V(1) - U_0(1) - \tau_- U_+(1) - \tau_+ U_-(1) \right. \\
 & \left. - \tau_3 U_3(1) \right] \delta^{(4)}(1-1') \\
 & + i \int d^4 T \mathcal{V}(1-T) [\text{tr } G(TT^\dagger)] \delta^{(4)}(1-1') \\
 & + i \int d^4 T \int d^4 T' \mathcal{V}(1-T) G(1T') \Gamma_0(T'1'; T) \quad (3.1.7)
 \end{aligned}$$

To make use of the variational derivative technique, the expressions (3.1.2) will now be recast in terms of suitable derivatives. For,

$$\langle \sigma_i(1) \rangle = -i [\text{tr } \tau_i G(11^\dagger)] \quad (i = 0, 1, 2, 3)$$

where 1, 2, 3 now refer to spherical components (+, -, 3). So one has,

$$\begin{aligned}
 - \frac{\delta}{\delta U_j(2)} [\text{tr } \tau_i G(11^\dagger)] &= \langle T(\sigma_i(1) \sigma_j(2)) \rangle - \langle \sigma_i(1) \rangle \langle \sigma_j(2) \rangle \\
 &= \langle T((\sigma_i(1) - \langle \sigma_i(1) \rangle) (\sigma_j(2) - \langle \sigma_j(2) \rangle)) \rangle \\
 &= \langle T(\hat{\sigma}_i(1) \hat{\sigma}_j(2)) \rangle
 \end{aligned}$$

Also

$$\frac{\delta G(11^\dagger)}{\delta U_j(2)} = - \int d^4 \bar{2} d^4 \bar{3} G(1\bar{2}) \Gamma_j(\bar{2}\bar{3}; 2) G(\bar{3}1(t_1^\dagger)) \quad (3.1.9)$$

from (2.1.25), and ^{after} defining

$$\Gamma_j(12; 3) = \delta G^{-1}(12)/\delta U_j(3) \quad (3.1.10)$$

The Γ_j are matrices like Γ_0 in the last chapter. Hence

$$\chi_{ij}(12) = i \int d^4\bar{T} d^4\bar{Z} [\text{tr} \{ \tau_i G(1\bar{T}) \Gamma_j(\bar{T}\bar{Z}; 2) G(\bar{Z}1(t_1^+)) \}] \quad (3.1.11)$$

The equations for Γ_j can now be written down with the help of (3.1.7)

$$\begin{aligned} \Gamma_j(12; 3) = & -\tau_j \delta^{(4)}(1-2) \delta^{(4)}(1-3) - \\ & - i \int d^4\bar{T} d^4\bar{Z} d^4\bar{3} \mathcal{V}(1-\bar{T}) [\text{tr} \{ G(\bar{T}\bar{Z}) \Gamma_j(\bar{Z}\bar{3}; 3) G(\bar{3}\bar{T}(t_1^+)) \}] \delta^{(4)}(1-2) - \\ & - i \int d^4\bar{T} d^4\bar{T}' d^4\bar{Z} d^4\bar{3} \mathcal{V}(1-\bar{T}) G(1\bar{Z}) \Gamma_j(\bar{Z}\bar{3}; 3) G(\bar{3}\bar{T}') \Gamma_0(\bar{T}2; \bar{T}) + \\ & + i \int d^4\bar{T} d^4\bar{T}' \mathcal{V}(1-\bar{T}) G(1\bar{T}') \frac{\delta \Gamma_0(\bar{T}2; \bar{T})}{\delta U_j(3)} \end{aligned} \quad (3.1.12)$$

These equations are exact. From (3.1.12) one can derive the equations for $\delta \Gamma_0/\delta U_j$ and so on. These form a set of linear equations for $\Gamma_1, \Gamma_2, \Gamma_3$ except that these are all coupled to Γ_0 which satisfies a nonlinear equation. The second term in (3.1.12) has an obvious interpretation and lets us introduce

$$\gamma_j(12) = i \int d^4\bar{T} d^4\bar{Z} [\text{tr} \{ G(1\bar{T}) \Gamma_j(\bar{T}\bar{Z}; 2) G(\bar{Z}1(t_1^+)) \}] \quad (3.1.13)$$

This term arises from the Hartree term in G^{-1} , the next to last term in (3.1.7), and has, therefore, the interpretation that it is the response of the total particle density to the component U_i of the external field

$$\gamma_i(12) = \frac{1}{i} \langle T(\rho(1), \hat{\sigma}_i(2)) \rangle \quad (3.1.14)$$

The various terms in (3.1.12) may be interpreted as follows. The first term is the lowest order HF term since in the last chapter this term was seen to give the conventional HF single particle excitations. The second term is due to direct scattering processes involving fluctuations in the Hartree self energy; the third term arises from the exchange scattering processes and the last term includes all the higher-order vertex corrections coming from various other scattering processes. The Eq. (3.1.12) in its full generality is very complicated and simplifying approximations have to be made. These will be discussed in the next section as well as the results obtained therefrom.

2. Approximations (Spatially Uniform Solutions)

We now consider the free gas where the single particle potential is taken to be zero. Then we have a spatially uniform system where the Green's function $G(11')$ depends only on the difference $(1-1')$ and the functions $\Gamma_i(12; 3)$ depend only on $(1-2)$ and $(1-3)$. Before proceeding further, we note that the last term in (3.1.12) is of order v^2 as can be seen by forming the equation for $\delta\Gamma_0/\delta U_i$. We, therefore, drop this term in all our calculations. This amounts to neglecting all vertex corrections. (See, for example, Rajagopal [45] for a discussion of these equations in the extended RPA scheme using the above formalism.) We now take the Fourier transform of this using (2.2.1) and (2.5.4) where 4-D notation is used for convenience.

$$\Gamma_i(k; q) = -\tau_i - \mathcal{V}(q) \gamma_i(q) - i \int \mathcal{V}(k - \bar{q}) G(q + \bar{q}) \cdot$$

$$\Gamma_i(\bar{q}; q) G(\bar{q}) \Gamma_o(k; \bar{q} - k) \frac{d^4 \bar{q}}{(2\pi)^4} \quad (3.2.1)$$

$\gamma_i(q)$ is just the Fourier transform of (3.1.14) and has the form

$$\gamma_i(q) = i \int \frac{d^4 \bar{q}}{(2\pi)^4} [\text{tr} \{ G(q + \bar{q}) \Gamma_i(\bar{q}; q) G(\bar{q}) \}] \quad (3.2.2)$$

From the structure of (3.2.1), following a suggestion used in another context by Nambu [43], an algebraic transformation may be made:

$$\Gamma_i(k; q) = \Lambda_i(k; q) + \mathcal{V}(q) \gamma_i(q) \Lambda_o(k; q) \quad (3.2.3)$$

where now

$$\Lambda_i(k; q) = -\tau_i - i \int \frac{d^4 \bar{q}}{(2\pi)^4} \mathcal{V}(k - \bar{q}) G(q + \bar{q}) \Lambda_i(\bar{q}; q) G(\bar{q}) \Gamma_o(k; \bar{q} - k) \quad (3.2.4)$$

In view of (3.2.3), one has the form

$$\gamma_i(q) = i \int \frac{d^4 \bar{q}}{(2\pi)^4} [\text{tr} \{ G(q + \bar{q}) \Lambda_i(\bar{q}; q) G(\bar{q}) \}] / \mathcal{E}(q) \quad (3.2.5)$$

with

$$\mathcal{E}(q) = 1 -$$

$$-i \mathcal{V}(q) \int \frac{d^4 \bar{q}}{(2\pi)^4} [\text{tr} \{ G(q + \bar{q}) \Lambda_o(\bar{q}; q) G(\bar{q}) \}] \quad (3.2.6)$$

But $\gamma_0(q)$ is the Fourier transform of the density correlation function, and so one has the following general relationship between $\epsilon(q)$ and $\gamma_0(q)$ which is obtained from their definitions (3.2.5, 6) :

$$\gamma_0(q) = \frac{1}{\mathcal{V}(q)} \left[\frac{1}{\epsilon(q)} - 1 \right] \quad (3.2.7)$$

Comparing with (2.50) of Pines [32] (page 41), one thus sees that $\epsilon(q)$ may be identified with a propagating dielectric constant of the medium. In view of the definition (3.2.6), the equation for Γ_0 (cf. (3.2.3)) may be rewritten:

$$\Gamma_0(k; q) = \Lambda_0(k; q) / \epsilon(q) \quad (3.2.8)$$

and the equation (3.2.4) for Λ_i :

$$\begin{aligned} \Lambda_i(k; q) = & -\tau_i - \\ & - i \int \frac{d^4 \bar{q}}{(2\pi)^4} \frac{\mathcal{V}(k - \bar{q})}{\epsilon(\bar{q} - k)} G(q + \bar{q}) \Lambda_i(\bar{q}; q) G(\bar{q}) \Lambda_0(k; \bar{q} - k) \quad (3.2.9) \end{aligned}$$

Then one finally arrives at

$$\begin{aligned} \chi_{33} = & i \int \frac{d^4 \bar{q}}{(2\pi)^4} [\text{tr} \{ \tau_3 G(q + \bar{q}) \Lambda_3(\bar{q}; q) G(\bar{q}) \}] + \\ & + i \mathcal{V}(q) \gamma_3(q) \int \frac{d^4 \bar{q}}{(2\pi)^4} [\text{tr} \{ \tau_3 G(q + \bar{q}) \Lambda_0(\bar{q}; q) G(\bar{q}) \}] \quad (3.2.10) \end{aligned}$$

$$\begin{aligned} \chi_{+-} = & i \int \frac{d^4 \bar{q}}{(2\pi)^4} [\text{tr} \{ \tau_1 G(q + \bar{q}) \Lambda_2(\bar{q}; q) G(\bar{q}) \}] + \\ & + i \mathcal{V}(q) \gamma_2(q) \int \frac{d^4 \bar{q}}{(2\pi)^4} [\text{tr} \{ \tau_1 G(q + \bar{q}) \Lambda_0(\bar{q}; q) G(\bar{q}) \}] \quad (3.2.11) \end{aligned}$$

In this technique the dielectric screening of the exchange term, namely in the second term of (3. 2. 9), comes about quite naturally without any ad hoc assumptions. Moreover, a perturbative type of solution of the Λ_i equation in powers of the interaction strength gives the results of the extended RPA [45]. We will now present four cases, three of which depend on further simplifying approximations of the equations (3. 2. 9).

To motivate the approximations, let us examine how the terms in (3. 2. 9) came about. To this end, the expression (2. 5. 5) for $G^{-1}(k)$ with all the $U_i = 0$, must be seen. This contains a term involving Γ_0 , or equivalently Λ_0 . It is this which couples the various Γ_i to Γ_0 as well as making the equation for Γ_0 nonlinear. However, the Γ_0 equation is inhomogeneous. It was earlier seen that taking the inhomogeneous term for Γ_0 to be the solution gives the HF approximation for G . So, if the equations for Γ_i or equivalently for Λ_i are derived from G_{HF} , one will arrive at equations of the form (3. 2. 1), but in the last term, Γ_0 appearing at the end is set equal to -1 thus

$$\begin{aligned} \Gamma_i(k; q) = & -\tau_i - \mathcal{V}(q) \gamma_i(q) + \\ & + i \int \frac{d^4 \bar{q}}{(2\pi)^4} \mathcal{V}(k - \bar{q}) G(q + \bar{q}) \Gamma_i(\bar{q}; q) G(\bar{q}). \end{aligned} \quad (3.2.12)$$

And correspondingly

$$\begin{aligned} \Lambda_i(k; q) = & -\tau_i + \\ & + i \int \frac{d^4 \bar{q}}{(2\pi)^4} \mathcal{V}(k - \bar{q}) G(q + \bar{q}) \Lambda_i(\bar{q}; q) G(\bar{q}). \end{aligned} \quad (3.2.13)$$

These equations then constitute the usual RPA equations but include lowest order exchange terms and must be solved to arrive at the various response functions. Again, the equation for Λ_i as in (3.2.13) cannot be solved completely, but this time for a different reason. The lowest order RPA consists in taking the inhomogeneous term to be the solution for Λ_i . But this is the lowest order approximation when $\mathcal{V}(k)$ depends on k . On the other extreme, if $\mathcal{V}(k)$ is chosen to be independent of k , which is true for zero range interactions, then further, if G 's are assumed to be diagonal, (3.2.3) can be solved trivially for Λ_i . This then is the second case where some physically nontrivial results are obtained. In this way of treating the problem, it is thus seen that the results for the Coulomb gas and the zero range gas come about quite trivially. These will be discussed in the next two subsections. We henceforth assume the G 's to be diagonal.

There is another possibility in the present context. This is to consider the full set of equations for Λ_i and G^{-1} together. We assume $\Lambda_0 = -1$ to start with. This is substituted in the expression for $\mathcal{E}(q)$ which now becomes the RPA dielectric constant. This, therefore, screens the exchange term in G^{-1} . The resulting equations for Λ_i ($i = 1, 2, 3$) are now independent of Λ_0 but are of the form (3.2.13) where in the last term, the interaction potential is screened by \mathcal{E}_{RPA} . This new set will be discussed to justify the use of the Yukawa potential in this problem. This is discussed as Case (c). After describing these results, in the next section, the results are extended to Bloch electrons, which form the fourth case of the present discussion.

It may be mentioned in passing that the same method was employed by the author [46] to derive quite trivially the dielectric constant of an electron gas in the presence of an external magnetic field.

A. Coulomb Gas

Here $\mathcal{V}(q) = \frac{4\pi e^2}{q^2}$ and only the most trivial approximations can be made to give closed form results. Here the solutions to (3.2.13) are taken to be

$$\Lambda_i^I(k; q) = -\tau_i \quad (3.2.14)$$

Then

$$\epsilon_I(q) = 1 + \mathcal{V}(q) (A_I + B_I) \quad (3.2.15a)$$

$$\gamma_0^I(q) = - \left[\frac{(A_I + B_I)}{1 + \mathcal{V}(q) (A_I + B_I)} \right] \quad (3.2.15b)$$

$$\gamma_1^I(q) = 0 \quad (3.2.15c)$$

$$\gamma_2^I(q) = 0 \quad (3.2.15d)$$

$$\gamma_3^I(q) = - \left[\frac{(A_I - B_I)}{1 + \mathcal{V}(q) (A_I + B_I)} \right] \quad (3.2.15e)$$

$$\chi_{33}^I(q) = - \left[\frac{A_I + B_I + 4\mathcal{V}(q) A_I B_I}{1 + \mathcal{V}(q) (A_I + B_I)} \right] \quad (3.2.15f)$$

$$\chi_{+-}^I(q) = -C_I \quad (3.2.15g)$$

Here

$$A_I = i \int \frac{d^4 \bar{q}}{(2\pi)^4} G_{\uparrow\uparrow}(q + \bar{q}) G_{\uparrow\uparrow}(\bar{q}) \quad (3.2.16a)$$

$$B_I = i \int \frac{d^4 \bar{q}}{(2\pi)^4} G_{\uparrow\downarrow}(q + \bar{q}) G_{\uparrow\downarrow}(\bar{q}) \quad (3.2.16b)$$

$$C_I = i \int \frac{d^4 \bar{q}}{(2\pi)^4} G_{\downarrow\downarrow}(q + \bar{q}) G_{\downarrow\downarrow}(\bar{q}) \quad (3.2.16c)$$

Integrals of the type (3.2.16a, b, c) with the same general structure will appear in the future also. Using a method given in KB, these can be evaluated in general in the form:

$$A(q\omega) = \int \frac{d^3 \bar{q}}{(2\pi)^3} \int \frac{d\bar{\omega}}{2\pi} \int \frac{d\bar{\omega}}{2\pi} \frac{A_{\uparrow\uparrow}(q + \bar{q}; \bar{\omega}) A_{\uparrow\uparrow}(\bar{q}; \bar{\omega})}{\omega - \bar{\omega} + \bar{\omega}} (n_F(\bar{\omega}) - n_F(\bar{\omega})) \quad (3.2.17a)$$

$$B(q\omega) = \int \frac{d^3 \bar{q}}{(2\pi)^3} \int \frac{d\bar{\omega}}{2\pi} \int \frac{d\bar{\omega}}{2\pi} \frac{A_{\uparrow\downarrow}(q + \bar{q}; \bar{\omega}) A_{\uparrow\downarrow}(\bar{q}; \bar{\omega})}{\omega - \bar{\omega} + \bar{\omega}} (n_F(\bar{\omega}) - n_F(\bar{\omega})) \quad (3.2.17b)$$

$$C(q\omega) = \int \frac{d^3 \bar{q}}{(2\pi)^3} \int \frac{d\bar{\omega}}{2\pi} \int \frac{d\bar{\omega}}{2\pi} \frac{A_{\downarrow\downarrow}(q + \bar{q}; \bar{\omega}) A_{\downarrow\downarrow}(\bar{q}; \bar{\omega})}{\omega - \bar{\omega} + \bar{\omega}} (n_F(\bar{\omega}) - n_F(\bar{\omega})) \quad (3.2.17c)$$

The weight functions $A_{\sigma\sigma'}$ are as given in Chapter II. The HF approximation gives

$$A_{\uparrow\uparrow}(q\omega) = 2\pi \delta(\omega - \epsilon_{\uparrow}^{HF}(q)); \quad A_{\uparrow\downarrow}(q\omega) = 2\pi \delta(\omega - \epsilon_{\downarrow}^{HF}(q)) \quad (3.2.18)$$

These in (3.2.17) give the combination

$$[n_F(\epsilon_{\sigma}^{HF}(q + \bar{q})) - n_F(\epsilon_{\sigma'}^{HF}(\bar{q}))]$$

of Fermi functions. We take this to be

$$[\eta_+(k_{F\sigma} - |q + \bar{q}|) - \eta_+(k_{F\sigma} - |\bar{q}|)]$$

for $T = 0^\circ\text{K}$ as in (2.5.8). Note that these integrals in general have a principal part and a delta function part or in other words they have real and imaginary parts. For the present case:

$$A_I = \int \frac{d^3\bar{q}}{(2\pi)^3} \left[\frac{n_F(\omega_+^I(q + \bar{q})) - n_F(\omega_+^I(\bar{q}))}{\omega - \omega_+^I(q + \bar{q}) + \omega_+^I(\bar{q})} \right] \quad (3.2.19a)$$

$$B_I = \int \frac{d^3\bar{q}}{(2\pi)^3} \left[\frac{n_F(\omega_-^I(q + \bar{q})) - n_F(\omega_-^I(\bar{q}))}{\omega - \omega_-^I(q + \bar{q}) + \omega_-^I(\bar{q})} \right] \quad (3.2.19b)$$

$$C_I = \int \frac{d^3\bar{q}}{(2\pi)^3} \left[\frac{n_F(\omega_-^I(q + \bar{q})) - n_F(\omega_+^I(\bar{q}))}{\omega - \omega_-^I(q + \bar{q}) + \omega_+^I(\bar{q})} \right] \quad (3.2.19c)$$

with

$$\omega_{\pm}^I(q) = q^2/2m -$$

$$- \left(\frac{e^2}{\pi q} \right) \left[qk_{F\sigma} + \frac{1}{2} (q^2 - k_{F\sigma}^2) \ln \left| \frac{q - k_{F\sigma}}{q + k_{F\sigma}} \right| \right] \quad (3.2.20)$$

Here $k_{F\sigma}$: + corresponds to $k_{F\uparrow}$; - to $k_{F\downarrow}$

The expression for $\epsilon_I(q)$ derived under these approximations corresponds to the dielectric constant derived by various authors within the RPA (see Pines [32]) in the unpolarized limit. We will, therefore, call this plasma RPA.

One notices from the form of the Eq. (3.2.13) and the solution assumed (3.2.14) that the exchange terms are entirely neglected in this plasma RPA. Because of this the polarized system behaves as though one had just two non-interacting plasmas and the medium shows no spin wave mode in χ_{+-} . However, on taking the exchange terms into account by examining the Γ_2 equation in more detail, as will be done later, spin waves do result. (As a check on the calculations, if the system were unpolarized, $A = B = C$, the above results reduce to the known results found in the literature.) In this approximation, $\gamma_1(q) = \gamma_2(q) = 0$; this implies that there are no density fluctuations caused by the fluctuations of the transverse components of the internal polarization. However, $\gamma_3 \neq 0$, showing that the longitudinal component does affect the density. These results are reasonable on physical grounds also. In the complete F state, $B = 0$, (\downarrow state is empty) there is still a plasma type excitation found in both the density response and in χ_{33} . (The complete F state corresponds to an electron gas with one spin state occupied; two particles cannot come to the same spot ~~both~~ by dint of the Pauli principle. This is significant as will be seen in case (B).)

As a further crude approximation, to illustrate the results obtained so far, if the exchange terms in (3.2.20) are expanded for small q , one obtains an effective quadratic dispersion for the single particle energies with some effective masses:

$$\omega_{\pm}(q) = q^2/2m_{\sigma} - \frac{2e^2 k_{F\sigma}}{\pi} \quad \text{with} \quad \frac{1}{m_{\sigma}} = \left(\frac{1}{m} + \frac{4e^2}{3\pi k_{F\sigma}} \right) \quad (3.2.21)$$

This is only to give a heuristic argument. A more useful but perhaps irrelevant approximation is just to assume a quadratic dispersion law for the two states with effective masses, but without the significance of (3.2.21). In any case, one has plasma oscillations in the medium, appearing in the density response, γ_0 , $\gamma_3(q)$, and in χ_{33} . In the P state, the plasma mode appears only in $\gamma_0(q)$.

We now derive the Thomas-Fermi screening in the polarized medium, using an effective mass approximation, for the \uparrow and \downarrow bands. For this we need to study $\mathcal{E}(\underline{q}, \omega=0)$ at $T = 0^\circ\text{K}$ for $q \sim 0$. We then have

$$\mathcal{E}(\underline{q}, \omega=0) = 1 + \frac{4\pi e^2}{q^2} \left\{ 2m_{\uparrow} \int \frac{d^3\bar{q}}{(2\pi)^3} \frac{\eta_+(k_{F\uparrow} - |\underline{q} + \bar{q}|) - \eta_+(k_{F\uparrow} - |\bar{q}|)}{|\underline{q} + \bar{q}|^2 - \bar{q}^2} + \right. \\ \left. + 2m_{\downarrow} \int \frac{d^3\bar{q}}{(2\pi)^3} \frac{\eta_+(k_{F\downarrow} - |\underline{q} + \bar{q}|) - \eta_+(k_{F\downarrow} - |\bar{q}|)}{|\underline{q} + \bar{q}|^2 - \bar{q}^2} \right\}.$$

Evaluating the integrals for small q , one has

$$\mathcal{E}(\underline{q}, \omega=0) = 1 + \frac{4\pi e^2}{q^2} \left(\frac{m_{\uparrow} k_{F\uparrow}^2}{2\pi^2} + \frac{m_{\downarrow} k_{F\downarrow}^2}{2\pi^2} \right) \\ = 1 + \xi_{TF}^2(\xi) k_F^2 / q^2$$

where

$$\xi_{TF}^2(\xi) = \frac{2}{\pi} (\text{ar}_s) \left[\frac{m_{\uparrow}}{m} (1+\xi)^{1/3} + \frac{m_{\downarrow}}{m} (1-\xi)^{1/3} \right] \quad (3.2.22)$$

Here m_{σ} are taken to be arbitrary. Using $m_{\uparrow} = m_{\downarrow} = m$, we have plotted in Fig. 2a $\xi(\xi=0, 1)$ versus $\ln(ar_g)$ to show where the Thomas-Fermi screening lies on the phase plot of HF ground states for the Yukawa potential. This shows that ferromagnetism does not occur in HF for Thomas-Fermi screening.

B. Zero-Range Gas (Stoner model)

Here $\mathcal{V}(q) = \overline{\mathcal{V}} = \text{a constant}$. In this case, the equations for Λ_i can all be solved trivially if the G 's are diagonal. These are:

$$\Lambda_0^{\text{II}}(k; q) = - \begin{pmatrix} 1/(1 - \overline{\mathcal{V}}A_{\text{II}}) & 0 \\ 0 & 1/(1 - \overline{\mathcal{V}}B_{\text{II}}) \end{pmatrix} \quad (3.2.23a)$$

$$\Lambda_1^{\text{II}}(k; q) = -\tau^+ (1/(1 - \overline{\mathcal{V}}D_{\text{II}})) \quad (3.2.23b)$$

$$\Lambda_2^{\text{II}}(k; q) = -\tau^- (1/(1 - \overline{\mathcal{V}}C_{\text{II}})) \quad (3.2.23c)$$

$$\Lambda_3^{\text{II}}(k; q) = - \begin{pmatrix} 1/(1 - \overline{\mathcal{V}}A_{\text{II}}) & 0 \\ 0 & -1/(1 - \overline{\mathcal{V}}B_{\text{II}}) \end{pmatrix} \quad (3.2.23d)$$

where $D_{\text{II}} = i \int \frac{d^4\bar{q}}{(2\pi)^4} G_{\uparrow\uparrow}(q+\bar{q}) G_{\downarrow\downarrow}(\bar{q})$.

Then

$$\gamma_0^{\text{II}}(q) = - \frac{1}{\mathcal{E}_{\text{II}}(q)} \left[\frac{A_{\text{II}} + B_{\text{II}} - 2\overline{\mathcal{V}}A_{\text{II}}B_{\text{II}}}{(1 - \overline{\mathcal{V}}A_{\text{II}})(1 - \overline{\mathcal{V}}B_{\text{II}})} \right] \quad (3.2.24a)$$

$$\epsilon_{II}^{\text{II}}(q) = + \left[\frac{1 - \bar{\nu}^2 A_{II} B_{II}}{(1 - \bar{\nu} A_{II})(1 - \bar{\nu} B_{II})} \right] \quad (3.2.24b)$$

and hence

$$\gamma_0^{\text{II}}(q) = - \left[\frac{A_{II} + B_{II} - 2\bar{\nu} A_{II} B_{II}}{1 - \bar{\nu}^2 A_{II} B_{II}} \right] \quad (3.2.24a')$$

$$\gamma_1^{\text{II}}(q) = 0 \quad (3.2.24c)$$

$$\gamma_2^{\text{II}}(q) = 0 \quad (3.2.24d)$$

$$\gamma_3^{\text{II}}(q) = - \left[\frac{A_{II} - B_{II}}{1 - \bar{\nu}^2 A_{II} B_{II}} \right] \quad (3.2.24e)$$

$$\chi_{33}^{\text{II}}(q) = - \left[\frac{A_{II} + B_{II} + 2\bar{\nu} A_{II} B_{II}}{1 - \bar{\nu}^2 A_{II} B_{II}} \right] \quad (3.2.24f)$$

$$\chi_{+-}^{\text{II}}(q) = - C_{II} / (1 - \bar{\nu} C_{II}). \quad (3.2.24g)$$

$$\begin{aligned} \omega_{\pm}^{\text{II}} &= q^2/2m - \frac{1}{2} N \bar{\nu} (1 \pm \xi) \\ &= q^2/2m - K\theta' (1 \pm \xi) \text{ in Stoner's notation} \end{aligned} \quad (3.2.25)$$

As with the results of case (A), γ_0^{II} , γ_3^{II} , and χ_{33}^{II} show the same pole structure. However, χ_{+-}^{II} contains a pole also, showing the possibility of spin-wave modes in the medium without additional approximations. In the paramagnetic limit, $A_{II} = B_{II} = C_{II}$; γ_0^{II} contains a pole while χ_{33}^{II} has none, for repulsive potential. In this limit, the results correspond to those

of Gottfried and Pigman [30] and Wolff [31], respectively. If one puts $\mathcal{V}(q) = \overline{\mathcal{V}}$ in the results of case (A), in the P state, one finds it necessary to take $\mathcal{V}(q) \sim \overline{\mathcal{V}}/2$ to find results in agreement with those of the present section. This factor of $\frac{1}{2}$ appears because the exchange contributions were neglected in case (A) and were taken into account here. For the same reason, the substitution $\mathcal{V}(q) = \overline{\mathcal{V}}$ in case (A) does not give the same results as case (B) in the polarized case. The appearance of spin waves as a pole in χ_{+-}^{II} is entirely due to exchange. The above results have also been derived by Kubo et.al. [26] and Baym [27]. As in (A), $\gamma_1 = \gamma_2 = 0$ for the same reason.

The integrals can all be formally reduced to quadratures for finite T, and to closed expressions for $T = 0^\circ\text{K}$, thus (only principal parts are here given):

$$\left. \begin{aligned} A_{\text{II}} &= -\frac{m}{4\pi^2 q} \int dq' q' n_F(\omega_+^{\text{II}}(q')) \ln \left[\frac{\omega^2 - (q^2/2m - qq'/m)^2}{\omega^2 - (q^2/2m + qq'/m)^2} \right] \\ B_{\text{II}} &= -\frac{m}{4\pi^2 q} \int dq' q' n_F(\omega_-^{\text{II}}(q')) \ln \left[\frac{\omega^2 - (q^2/2m - qq'/m)^2}{\omega^2 - (q^2/2m + qq'/m)^2} \right] \\ C_{\text{II}} &= -\frac{m}{4\pi^2 q} \int dq' q' \left\{ n_F(\omega_-^{\text{II}}(q')) \ln \left[\frac{\overline{\Omega} + q^2/2m - qq'/m}{\overline{\Omega} + q^2/2m + qq'/m} \right] - \right. \\ &\quad \left. - n_F(\omega_+^{\text{II}}(q')) \ln \left[\frac{\overline{\Omega} - q^2/2m - qq'/m}{\overline{\Omega} - q^2/2m + qq'/m} \right] \right\} \end{aligned} \right\} \quad (3.2.26)$$

$$\overline{\Omega} = (\omega - 2K\theta' \zeta).$$

(3.2.26)

For $T = 0^\circ\text{K}$, these integrals can be carried out and are:

$$\begin{aligned}
 A_{II} &= -\frac{m^3}{8\pi^2 q^3} \left\{ -2q^3 k_{F\uparrow} / m^2 + \right. \\
 &\quad + [(\omega + q^2/2m)^2 - q^2 k_{F\uparrow}^2 / m^2] \ln \left[\frac{\omega + q^2/2m + q k_{F\uparrow} / m}{\omega + q^2/2m - q k_{F\uparrow} / m} \right] - \\
 &\quad \left. - [(\omega - q^2/2m)^2 - q^2 k_{F\uparrow}^2 / m^2] \ln \left[\frac{\omega - q^2/2m + q k_{F\uparrow} / m}{\omega - q^2/2m - q k_{F\uparrow} / m} \right] \right\} \\
 B_{II} &= (\text{same as above with } k_{F\uparrow} \text{ replaced by } k_{F\downarrow}) \\
 C_{II} &= -\frac{m^3}{8\pi^2 q^3} \left\{ \frac{2q}{m} [(\bar{\Omega} - q^2/2m) k_{F\uparrow} - (\bar{\Omega} + q^2/2m) k_{F\downarrow}] + \right. \\
 &\quad + [(\bar{\Omega} + q^2/2m)^2 - q^2 k_{F\downarrow}^2 / m^2] \ln \left[\frac{\bar{\Omega} + q^2/2m + q k_{F\downarrow} / m}{\bar{\Omega} + q^2/2m - q k_{F\downarrow} / m} \right] - \\
 &\quad \left. - [(\bar{\Omega} - q^2/2m)^2 - q^2 k_{F\uparrow}^2 / m^2] \ln \left[\frac{\bar{\Omega} - q^2/2m + q k_{F\uparrow} / m}{\bar{\Omega} - q^2/2m - q k_{F\uparrow} / m} \right] \right\}
 \end{aligned} \tag{3.2.27}$$

These principal parts are evaluated here so that when the imaginary parts of these integrals vanish (which they do for a certain range of the q vector specified by the logarithmic singularities in (3.2.27)), they directly give the information concerning the real poles in the ω -plane. These real poles in the correlation function correspond to resonant bound states. When the imaginary parts of these integrals are finite, the reality of ω is lost; the bound states have finite lifetimes in these approximations. The physical mechanism for these lifetimes has already been outlined in Chapter I, and will not be repeated here.

For small q , these expressions can be further simplified by making approximate evaluations:

$$A_{II} \sim -q^2 N_{\uparrow} / m\omega^2; \quad B_{II} \sim -q^2 N_{\downarrow} / m\omega^2. \quad (3.2.28)$$

The evaluation of C_{II} for this limit is a little more subtle because of the presence of $2K\theta'\zeta$. Writing $\bar{\Omega} = (\omega - 2K\theta'\zeta)$ it is here given up to order $(q^2/\bar{\Omega}^3)$ the reason for which becomes evident when the spin-wave pole is evaluated.

$$C_{II} \sim -\frac{\xi k_F^3}{3\pi^2 \bar{\Omega}^3} \left\{ \bar{\Omega}^2 + \frac{q^2 \bar{\Omega}}{2m\xi} + \frac{q^2 k_F^2}{10m^2 \xi} [(1+\xi)^{5/3} - (1-\xi)^{5/3}] \right\}. \quad (3.2.29)$$

The poles of γ_0^{II} , γ_3^{II} , and χ_{33}^{II} are of the form

$$1 - \bar{\nu}^2 A_{II} B_{II} = 0 \doteq 1 - \bar{\nu}^2 q^4 N_{\uparrow} N_{\downarrow} / m^2 \omega^4$$

or

$$\omega \doteq \left(\frac{\bar{\nu}^2 N_{\uparrow} N_{\downarrow}}{m^2} \right)^{1/4} q. \quad (3.2.30)$$

There is thus a sound mode in the medium traveling with a velocity given by

$$(\bar{\nu} N / 2m)^{1/2} (1-\xi^2)^{1/4} \quad \text{or} \quad v_F \left(\frac{K\theta'}{2\epsilon_F} \right)^{1/2} (1-\xi^2)^{1/4}$$

(v_F is the Fermi velocity k_F/m). For the P state, $K\theta'/\epsilon_F = 2/3$, this is $v_F/\sqrt{3}$ which is the usual result. It must be remarked here that in the F state, $B_{II} = 0$ (only \uparrow states are occupied) so that \mathcal{E}_{II} has no zeros or γ_0 has no poles showing that there is no sound mode propagation. However, the spin waves are seen to exist in this state. Note that a plasma mode did exist in the F state in the Coulomb case, in (A). This result will be

evident when the situation is visualized in some detail. In the case of zero-range interaction, the particles interact only when they are very close to each other. In the F state all the particles have up spin and so the Pauli principle comes into play and precludes the interactions entirely. (The sound mode is found in γ_0 , which, as was pointed out earlier, may be thought of as singlet state of the pair; in the present instance, no singlet state can be formed. This is another reason for not finding a sound mode in the medium.) The longitudinal susceptibility also does not show any resonant response (it did in the Coulomb case in (A)) because the spins are already lined up and no longitudinal field can fluctuate it any further because the interactions are of zero range. However, the transverse susceptibility shows the spin-wave mode as must be the case and as is reasonable otherwise. Note in this case, $\gamma_0^{II} = \gamma_3^{II} = \chi_{33}^{II} = -A_{II}$ which can be expected because $N = \sigma_3$ for, $N = N_{\uparrow} + N_{\downarrow} = N_{\uparrow}$ (F state) and $\sigma_3 = N_{\uparrow} - N_{\downarrow} = N_{\uparrow}$ (F state).

The spin-wave mode will now be discussed in some detail. This requires the evaluation of the zeros of $(1 - \bar{\mathcal{Q}}^1 C_{II})$ in the limit of small q and small ω , such that terms of order (ωq^2) and (ω^3) are neglected. Then one has

$$\omega_{SW} \sim \frac{q^2}{2m\xi(K\theta'/\epsilon_F)} \left[\frac{K\theta'}{\epsilon_F} - \frac{((1+\xi)^{5/3} - (1-\xi)^{5/3})}{5\xi} \right] \quad (3.2.31)$$

The stability of the spin-wave mode may be ascertained by imposing the condition that its frequency be positive. This criterion gives

$$K\theta'/\epsilon_F > [(1+\zeta)^{5/3} - (1-\zeta)^{5/3}]/5\zeta \quad (3.2.32)$$

For the fully ferromagnetic case this is

$$K\theta'/\epsilon_F > 2^{5/3}/5 \sim 0.635 \quad (3.2.33)$$

From Chapter II, the ground state is an F state if

$$K\theta'/\epsilon_F > 2^{-1/3} \sim 0.794 \quad (3.2.34)$$

and the ground state is UF if $K\theta'/\epsilon_F > 2/3 \sim 0.667$. Thus, whenever the ground state is either UF or F the spin waves are stable also. This was first noticed by Herring [23] and again recently by Fukuda [12].

There is a second type of instability of spin waves. Here the spin waves merge with the scattering states thus acquiring a finite lifetime even in RPA. This happens only beyond a certain maximum wave vector, q_{\max} of the spin wave, because X_{+-} will then have complex poles. The imaginary part of C_{II} begins to appear first for q_{\max} and ω_{SW} given by

$$\omega_{SW} = q_{\max}^2/2m + 2K\theta'\zeta - q_{\max}k_F/m \quad (3.2.35)$$

Calling $q_{\max} = Q_{\max} k_F$, one arrives at a transcendental equation for Q_{\max} , obtained by putting (3.2.35) in the spin-wave dispersion law $1 = \mathcal{D}C_{II}$ (3.2.27):

$$Q_{\max} = \frac{3}{8} (K\theta'/\epsilon_F) \left\{ 2(1+\xi)^{2/3} + 2(1-\xi)^{1/3} (Q_{\max}^{-(1+\xi)^{1/3}}) + \right. \\ \left. + [(Q_{\max}^{-(1+\xi)^{1/3}})^2 - (1-\xi)^{2/3}] \ln \left| \frac{Q_{\max}^{-(1+\xi)^{1/3}} - (1-\xi)^{1/3}}{Q_{\max}^{-(1+\xi)^{1/3}} + (1-\xi)^{1/3}} \right| \right\} \quad (3.2.26)$$

This has to be solved numerically. This numerical solution is displayed in Fig. 6. From (3.2.26) and from the schematic diagram in Fig. 6, it is seen that Q_{\max} has an upper bound at $(1+\xi)^{1/3} - (1-\xi)^{1/3}$. In this figure, $K\theta'/\epsilon_F$ is taken to be an independent parameter not determined by the ground state conditions. The only relevant parameter of course is the one pertaining to the ground state and the corresponding curve is shown in Fig. 6 as a broken-line curve. For $\xi = 1$, the F state, this gives an exact answer, namely

$$Q_{\max} = 3/2 (K\theta'/\epsilon_F) 2^{-1/3} \quad (3.2.27)$$

For such a Q_{\max} , the spin-wave frequency is

$$\omega_{SW}(Q_{\max} k_F) = \epsilon_F \left(\frac{K\theta'}{\epsilon_F} \right) \frac{9}{8} \cdot 2^{1/3} \left[\frac{K\theta'}{\epsilon_F} - \frac{4}{9} \cdot 2^{2/3} \right] \quad (3.2.28)$$

The spin-wave stability criterion applied to this shows that $\omega_{SW}^{\xi=1}(Q_{\max} k_F)$ is stable only if $K\theta'/\epsilon_F > 0.71$. This implies that for stable F states for which $K\theta'/\epsilon_F > 0.794$ the spin waves are stable up to Q_{\max} but beyond Q_{\max} they are unstable, being scattered into the individual particle excitations, even though the infinitesimal spin-wave stability criterion permits spin-waves to persist. If we take the stable F state for which $K\theta'/\epsilon_F = 2^{-1/3}$ (3.2.28) gives the spin waves up to $Q_{\max} = 0.945$ and its energy is $\omega_{SW}(q_{\max}) = 2^{2/3} \epsilon_F/16$ or $\epsilon_F/16$.

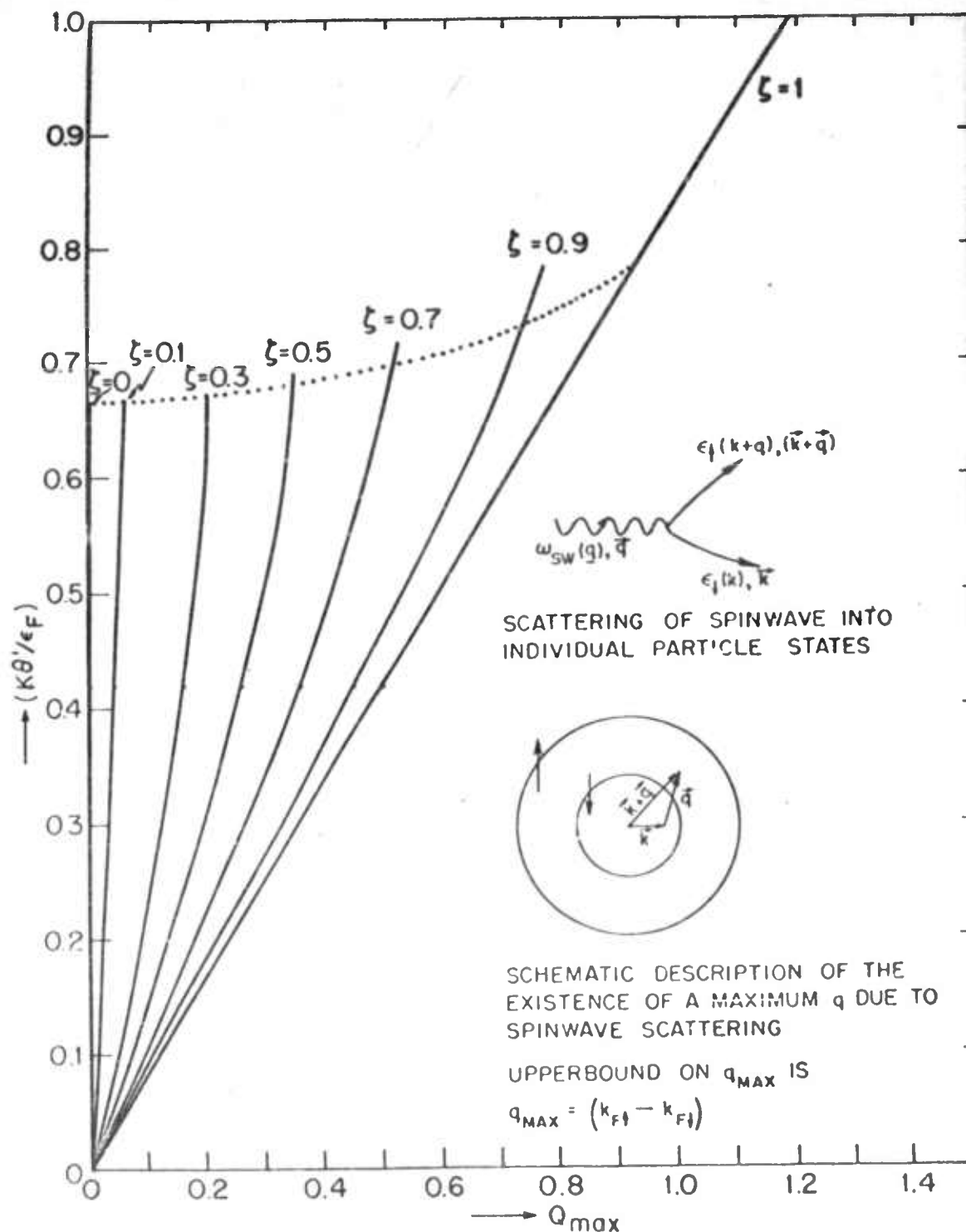


FIG. 6 Q_{max} vs. $K\theta'/\epsilon_F$ FOR VARIOUS ζ IN THE STONER MODEL. DOTTED-LINE CURVE REFERS TO $K\theta'/\epsilon_F$ CONSISTENT WITH THAT EVALUATED FOR THE GROUND STATE FOR VARIOUS ζ .

It must be mentioned that using an approximate method for evaluating the coefficient of q^2 for ω_{SW} Herring [23], Thompson [24], and Fukuda [12] had each obtained the same coefficient as given here for the F state. Thompson [24] had also derived a value of Q_{max} for the F state, in agreement with that given here. Baym [27] had only estimated this Q_{max} for $\xi \ll 1$ and arrived at a value of $Q_{max} = 2^{-1/3} (K\theta'/\epsilon_F)\xi$, which, as expected, is smaller than that for the F state. The schematic diagram of how Q_{max} comes about is given in Fig. 1a as well as Fig. 6 which has been explained already. In this connection, an aspect of finite temperatures must be mentioned. For this case, the integrals A, B, C all acquire finite imaginary parts and, hence, the collective modes or, in particular, the spin-wave mode, will be slightly damped. Physically this is reasonable for, at finite temperatures, particle-particle scatterings occurring into empty states below the top of the Fermi distribution are more frequent and these tend to destroy the coherence of the bound state.

In the light of these results, one may remark on the nature of the difficulty in computing the total magnetization of the system. We have two relations for calculating the magnetization:

$$\langle \sigma_3 \rangle = -i [\text{tr } \tau_3 G(11^+)]$$

and

$$\langle \sigma_3(1) \rangle \delta^{(3)}(1-2) = \langle [\sigma_+(1), \sigma_-(2)]_- \rangle$$

at equal times. The direct evaluation of $\langle \sigma_3 \rangle$ from the single particle Green's function in the interacting system is very hard and so may be used only for very approximate calculations at high temperatures where the

interactions do not contribute to spin waves. But at very low temperatures, the correlations are important and one may use the second relation which can be computed to a much higher accuracy than G . It is not clear at the present time how these two have to be reconciled to arrive at the correct evaluation of the magnetization valid at all temperatures. It is clearly beset with a considerable difficulty of self-consistency.

In the next section we will discuss the existence of spin waves in a Yukawa gas. This does not follow as directly from the equations as for the zero-range gas. One needs to resort to certain transformations of the given equations.

C. Yukawa Gas

Let us examine the Eq. (3.2.1)

$$\Gamma_i(k; q) = -\tau_i - \mathcal{V}(q) \gamma_i(q) - i \int \frac{d^4 \bar{q}}{(2\pi)^4} \frac{\mathcal{V}(k - \bar{q})}{\mathcal{E}(\bar{q} - k)} G(q + \bar{q}) \Gamma_i(\bar{q}; q) G(\bar{q}) \Lambda_0(k; \bar{q} - k) \quad (3.2.1')$$

where we have used $\Gamma_0 = \Lambda_0 / \mathcal{E}$. In this we take $\Lambda_0 = -1$, so that $\mathcal{E} = \mathcal{E}_{\text{RPA}}$, which when evaluated for $\omega = 0$ and for small wave vectors gives $\mathcal{E}_{\text{RPA}} \sim 1 + k_{\text{TF}}^2 / k^2$; k_{TF} is the usual Thomas-Fermi screening. Hence $\mathcal{V} / \mathcal{E}$ has the appearance of a Yukawa potential. Thus, the Yukawa potential can be used consistently with the ground-state properties in examining the collective excitations. In case (A), if exchange is taken into account by an extended RPA of the type suggested earlier, it shifts the

pole and also gives a finite lifetime to the collective states. This is as expected since taking into account more interactions would tend to degenerate the coherence of the bound state. The use of "plasma" RPA with a Yukawa potential, however, gives results very similar to those in case (A) - a plasma pole or a zero sound mode depending on whether the screening is small or large, the transition being gradual. But spin waves will not appear in this approximation. A more careful calculation involving the exchange contributions is needed to derive spin waves. The spin-wave problem is now examined here in detail.

To study the spin waves, we investigate the equation for Γ_2 and only the component $(\Gamma_2)_{\downarrow\uparrow}$ in this equation contains an inhomogeneous term, since the inhomogeneity is caused by the external field and we are seeking resonant response to an external field. Then equation (3.2.1') takes the form

$$(\mathcal{V}_y = \mathcal{V}_{\text{Yukawa}})$$

$$\Gamma_{2\downarrow\uparrow}(k; q) = -1 +$$

$$+ i \int \mathcal{V}_y(k-\bar{q}) G_{\downarrow\downarrow}(q+\bar{q}) \Gamma_{2\downarrow\uparrow}(\bar{q}; q) G_{\uparrow\uparrow}(\bar{q}) \frac{d^4 \bar{q}}{(2\pi)^4} . \quad (3.2.39)$$

To study the collective mode we have to consider the homogeneous counterpart of this equation which we will now examine. This is equivalent to studying the pole structure of χ_{+-} . From (3.1.12) if the usual RPA is used, with $\Gamma_0(12; 3)$

in the third term equal to $-\delta^{(4)}(1-2) \cdot \delta^{(4)}(1-3)$ and neglecting $\delta\Gamma_0/\delta U$, it can be easily verified that $\Gamma_1(12; 3)$ is of the form $\delta(t_1 - t_2) \Gamma_1'(12; 3)$ so that in Fourier space, one may assert that in (3.2.39), $\Gamma_2(k; q)$ is independent of k_0 , the frequency part of k . Then the \bar{q}_0 integration in (3.2.39) can be carried out, which is just C as in (3.2.17c):

$$\Gamma_{2\uparrow\uparrow}(k; q) = \int \frac{d^3\bar{q}}{(2\pi)^3} \mathcal{V}_Y(\underline{k} - \bar{q}) \left[\frac{n_F(\omega_-(q+\bar{q}) - n_F(\omega_+(\bar{q}))}{\omega - \omega_-(q+\bar{q}) + \omega_+(\bar{q})} \right] \Gamma_{2\uparrow\uparrow}(\bar{q}; q) \quad (3.2.40)$$

(homogeneous part of (3.2.39)) where $\omega_{\pm}(q)$ are evaluated with the Yukawa potential as in Chapter II (2.5.10). It is interesting to note that in the limit $\omega = 0$, $q = 0$ (in this order of limits), (3.2.40) becomes the ground state condition, namely (2.2.15). Hence, in the P state limit, the two equations should yield the same results. We now make an algebraic transformation

$$\Gamma_{2\uparrow\uparrow}(k; q) = [\omega - \omega_-(k+q) + \omega_+(k)] \bar{\Gamma}_{2\uparrow\uparrow}(k; q) \quad (3.2.41)$$

Then

$$(\omega - \omega_-(k+q) + \omega_+(k)) \bar{\Gamma}_{2\uparrow\uparrow}(k; q) = - \int \frac{d^3\bar{q}}{(2\pi)^3} \mathcal{V}_Y(\underline{k} - \bar{q}) (n_F(\omega_+(\bar{q})) - n_F(\omega_-(q+\bar{q}))) \bar{\Gamma}_{2\uparrow\uparrow}(\bar{q}; q) \quad (3.2.42)$$

$$\omega_{\pm}(k) = k^2/2m - \int \frac{d^3\bar{q}}{(2\pi)^3} \mathcal{V}_Y(\underline{k} - \bar{q}) n_{\sigma}(\bar{q}) \quad (3.2.43)$$

Fukuda [12] arrived at an equation of the form (3.2.42) using an equation of motion method for the spin flip operator in the RPA which involves the exchange term and he worked out the Coulomb case in the F state. The present approach follows a procedure somewhat similar to that of Fukuda in solving (3.2.42) for a Yukawa potential, but for all ξ and ξ .

We will first indicate how (3.2.42) can be solved for quite general \mathcal{V} and then specialize to the Yukawa potential. Let $y = k/k_F$, $\bar{y} = \bar{q}/k_F$, $x = q/k_F$, $\omega = (k_F^2/2m) v$ and $ar_s = mc^2/k_F$ and also choose x as the z axis of a reference coordinate system. Then, since $\cos \theta = (\frac{4\pi}{3})^{1/2} Y_{10}(\theta\phi)$, $Y_{lm}(\theta\phi)$ being the usual spherical harmonics, we have

$$\left\{ v - x^2 - 2xy \left(\frac{4\pi}{3}\right)^{1/2} Y_{10}(\hat{y}) + \left(\frac{ar_s}{2}\right) \int d^3\bar{y} V(|y-\bar{y}|) [n_F(\omega_-(x+\bar{y})) - n_F(\omega_+(\bar{y}))] \bar{\Gamma}_{2\frac{1}{2}}(y; x) \right\} \\ = \left(\frac{ar_s}{2}\right) \int d^3\bar{y} V(|y-\bar{y}|) [n_F(\omega_-(x+\bar{y})) - n_F(\omega_+(\bar{y}))] \bar{\Gamma}_{2\frac{1}{2}}(\bar{y}; x) \quad (3.2.44)$$

where we have written for convenience, $\mathcal{V}(y-\bar{y}) = \frac{4\pi e^2}{2k_F} V(|y-\bar{y}|)$. Let $x = 0$ in this. Multiplying the resulting expression through by $(n_F(\omega_-(y)) - n_F(\omega_+(y)))$ and integrating over y , we see that a solution exists with

$$v = 0 \quad \text{and} \quad \bar{\Gamma}_{2\frac{1}{2}}(y, 0) = \text{a constant} \quad (3.2.45)$$

Multiplying (3.2.44) through by $(n_F(\omega_-(y+x)) - n_F(\omega_+(y)))$ and integrating over y we get

$$\begin{aligned}
& (\nu - x^2) \int \frac{d^3 y}{(2\pi)^3} (n_F(\omega_-(x+y)) - n_F(\omega_+(y))) \bar{\Gamma}_{2\uparrow\uparrow}(y; x) \\
& - 2x \left(\frac{4\pi}{3}\right)^{1/2} \int \frac{d^3 y}{(2\pi)^3} y Y_{10}(\hat{y}) (n_F(\omega_-(x+y)) - n_F(\omega_+(y))) \bar{\Gamma}_{2\uparrow\uparrow}(y; x) + \\
& + \left(\frac{ar_s}{\pi^2}\right) \iint \frac{d^3 y d^3 \bar{y}}{(2\pi)^3} V(|y - \bar{y}|) (n_F(\omega_-(x+y)) - n_F(\omega_+(y))) (n_F(\omega_-(x+\bar{y})) - n_F(\omega_+(\bar{y}))) \\
& \quad \bar{\Gamma}_{2\uparrow\uparrow}(y; x) \\
& = \left(\frac{ar_s}{\pi^2}\right) \iint \frac{d^3 y d^3 \bar{y}}{(2\pi)^3} V(|y - \bar{y}|) (n_F(\omega_-(x+y)) - n_F(\omega_+(y))) (n_F(\omega_-(x+\bar{y})) - n_F(\omega_+(\bar{y}))) \\
& \quad \bar{\Gamma}_{2\uparrow\uparrow}(\bar{y}; x)
\end{aligned}$$

Interchanging \bar{y} and y in the RHS, since V is in general symmetric, this term cancels the last term on the LHS and hence one arrives at a general expression for ν for all x , ξ , and ζ :

$$\begin{aligned}
\nu = x^2 + 2x \left(\frac{4\pi}{3}\right)^{1/2} \int \frac{d^3 y}{(2\pi)^3} y Y_{10}(\hat{y}) [n_F(\omega_-(x+y)) - n_F(\omega_+(y))] \bar{\Gamma}_{2\uparrow\uparrow}(y; x) \\
- \int \frac{d^3 y}{(2\pi)^3} [n_F(\omega_-(x+y)) - n_F(\omega_+(y))] \bar{\Gamma}_{2\uparrow\uparrow}(y; x)
\end{aligned} \quad (3.2.46)$$

To find the coefficient of x^2 , we expand $(n_F(\omega_-(x+y)) - n_F(\omega_+(y)))$ and $\bar{\Gamma}_{2\uparrow\uparrow}(y; x)$ in powers of x taking note of (3.2.45)

$$\left. \begin{aligned}
n_F(\omega_-(x+y)) - n_F(\omega_+(y)) &= n^{(0)}(y) + \sum_{i=1}^{\infty} \sum_{l=0}^{\infty} x^i Y_{l0}(\hat{y}) n_l^{(i)}(y) \\
\bar{\Gamma}_{2\uparrow\uparrow}(y; x) &= \bar{\Gamma}_{2\uparrow\uparrow}^{(0)} + \sum_{j=1}^{\infty} \sum_{l'm'} x^j Y_{l'm'}(\hat{y}) \bar{\Gamma}_{2\uparrow\uparrow}^{(j)}{}_{l'm'}(y)
\end{aligned} \right\} \quad (3.2.47)$$

Only Y_{10} appears in the first expression as the left-hand side contains explicitly only $x \cdot y$ (or \hat{y}) while this is not so clear in the second expression.

Working then only to lowest order, we find

$$v \simeq x^2 + 2x^2 \left(\frac{4\pi}{3}\right)^{1/2} \left\{ \frac{\int y^3 n^{(0)}(y) \bar{\Gamma}_{2\frac{1}{2}}^{(1)}(y) dy + \bar{\Gamma}_{2\frac{1}{2}}^{(0)} \int y^3 n_1^{(1)}(y) dy}{4\pi \bar{\Gamma}_{2\frac{1}{2}}^{(0)} \int y^2 n^{(0)}(y) dy} \right\} \quad (3.2.48)$$

Now clearly at $T = 0^\circ K$,

$$\begin{aligned} n_F(\omega_-(x+y)) - n_F(\omega_+(y)) &= [n_F(\omega_-(y)) - n_F(\omega_+(y))] \\ &= -2 \left(\frac{4\pi}{3}\right)^{1/2} y Y_{10}(\hat{y}) \delta((1-\xi)^{2/3} - y^2) + \dots \end{aligned}$$

so that

$$n^{(0)}(y) = n_F(\omega_-(y)) - n_F(\omega_+(y))$$

and

$$n_1^{(1)}(y) = -2 \left(\frac{4\pi}{3}\right)^{1/2} y \delta((1-\xi)^{2/3} - y^2)$$

(3.2.49)

Choosing

$$\bar{\Gamma}_{2\frac{1}{2}}^{(0)} = (3/4\pi)^{1/2} (a r_s / \pi) \quad (3.2.50)$$

we finally get

$$\omega_{SW} = q^2 / 2m\xi \left\{ 1 - \left(\frac{\pi}{a r_s}\right) S(\xi, \xi) \right\}$$

with

$$S(\xi, \xi) = \int dy y^3 (n_F(\omega_-(y)) - n_F(\omega_+(y))) \bar{\Gamma}_{2\frac{1}{2}}^{(1)}(y)$$

(3.2.51)

Now our task is to find $\bar{\Gamma}_{2l+10}^{(1)}(y)$. This is done by using (3.2.47) in (3.2.44) after multiplying it by $[n_F(\omega_-(x+y)) - n_F(\omega_+(y))]$, along with the expansion

$$v = v_2 x^2 + \dots \quad (3.2.52)$$

and then equating the coefficients of like powers of x on both sides of the resulting expression. Before doing this, let us note that formally

$$V(|y-\bar{y}|) = \frac{1}{y\bar{y}} \sum_{l''=0}^{\infty} Q_{l''}(y; \bar{y}) \left(\frac{2l+1}{2} \right) P_{l''}(\mu) \quad (3.2.53)$$

where μ is the angle between y and \bar{y} . Using $\int_{-1}^{+1} P_l(\mu) P_{l'}(\mu) d\mu = \frac{2}{2l+1} \delta_{ll'}$ we find

$$\frac{1}{y\bar{y}} Q_l(y; \bar{y}) = \int_{-1}^{+1} d\mu P_l(\mu) V(|y-\bar{y}|) \quad (3.2.53a)$$

In (3.2.53), referring y and \bar{y} to a system where x is the z axis,

$$P_{l''}(\mu) = 4\pi \sum_{m''} \left(\frac{1}{2l+1} \right) Y_{l''m''}(y) Y_{l''m''}^*(\hat{\bar{y}})$$

so that (3.2.53) takes the form

$$V(|y-\bar{y}|) = \frac{2\pi}{y\bar{y}} \sum_{l''m''} Q_{l''}(y; \bar{y}) Y_{l''m''}(\hat{y}) Y_{l''m''}(\hat{\bar{y}}) \quad (3.2.54)$$

Here Y_{lm} 's are such that

$$\int d\hat{y} Y_{lm}(\hat{y}) Y_{l'm'}^*(\hat{y}) = \delta_{ll'} \delta_{mm'} \quad (3.2.55)$$

where $\int d\hat{y} = \int_{-1}^{+1} d\mu \int_0^{2\pi} d\phi$ as is usually taken. In the Yukawa case, (3.2.53a) takes a particularly simple form

$$\frac{1}{y\bar{y}} Q_l(y; \bar{y}) = \int_{-1}^{+1} d\mu \frac{P_l(\mu)}{[y^2 + \bar{y}^2 + \xi^2 - 2y\bar{y}\mu]}$$

But since $Q_l(t) =$ ~~Legendre~~ ^{Legendre} function of the second kind

$$= \frac{1}{2} \int_{-1}^{+1} d\mu \frac{P_l(\mu)}{t - \mu},$$

we find

$$Q_l(y; \bar{y}) = Q_l\left(\frac{y^2 + \bar{y}^2 + \xi^2}{2y\bar{y}}\right). \quad (3.2.56)$$

The expansion (3.2.53) was anticipated in view of this. Using these, we get for the coefficient of x

$$\begin{aligned} & -2y\left(\frac{4\pi}{3}\right)^{1/2} Y_{10}(\hat{y}) \bar{\Gamma}_{21}^{(0)} + 2\left(\frac{ar_s}{\pi y}\right) \sum_{l'm'} Y_{l'm'}(\hat{y}) \bar{\Gamma}_{21}^{(1)} \int \bar{y} n^{(0)}(\bar{y}) Q_0(y; \bar{y}) d\bar{y} \\ & = 2\left(\frac{ar_s}{\pi y}\right) \sum_{l'm'} Y_{l'm'}(\hat{y}) \int \bar{y} n^{(0)}(\bar{y}) Q_l(y; \bar{y}) \bar{\Gamma}_{21}^{(1)} \bar{\Gamma}_{l'm'}^{(1)}(\bar{y}) d\bar{y} \end{aligned} \quad (3.2.57)$$

Multiplying this through by $Y_{lm}^*(\hat{y})$ and integrating over \hat{y} , we get

$$\begin{aligned}
 & -2y\left(\frac{4\pi}{3}\right)^{1/2} \bar{\Gamma}_{2\frac{1}{2}}^{(0)} \delta_{l1} \delta_{m0} + 2\left(\frac{ar_s}{\pi y}\right) \left[\int \bar{y} n^{(0)}(\bar{y}) Q_0(y; \bar{y}) d\bar{y} \right] \bar{\Gamma}_{2\frac{1}{2}}^{(1)}(y) = \\
 & = 2\left(\frac{ar_s}{\pi y}\right) \int \bar{y} n^{(0)}(\bar{y}) Q_1(y; \bar{y}) \bar{\Gamma}_{2\frac{1}{2}}^{(1)}(\bar{y}) d\bar{y}. \quad (3.2.58)
 \end{aligned}$$

Note that for $l \neq 1$, $m \neq 0$, this gives homogeneous equations for $\bar{\Gamma}_{2\frac{1}{2}}^{(1)}$ which can, therefore, be taken to be zero without loss of generality. Also only $\bar{\Gamma}_{2\frac{1}{2}}^{(1)}(y)$ appears in the expression (3.2.51) for ω_{SW} . Thus, we consider the equation for $l=1$, $m=0$ only. Using (3.2.50) for $\bar{\Gamma}_{2\frac{1}{2}}^{(0)}$, we finally have

$$\begin{aligned}
 & -y^2 + \left(\int \bar{y} n^{(0)}(\bar{y}) Q_0(y; \bar{y}) d\bar{y} \right) \bar{\Gamma}_{2\frac{1}{2}}^{(1)}(y) = \\
 & = \int \bar{y} n^{(0)}(\bar{y}) Q_1(y; \bar{y}) \bar{\Gamma}_{2\frac{1}{2}}^{(1)}(\bar{y}) d\bar{y}. \quad (3.2.59)
 \end{aligned}$$

This equation must be solved for $\bar{\Gamma}_{2\frac{1}{2}}^{(1)}$ to arrive at an explicit expression for the coefficient of q^2 in ω_{SW} . Note that the above framework is so far independent of the choice of interaction, and hence, is a proof of the existence of spin waves for quite general interactions.

Now we will specialize V to be a Yukawa potential, so that (3.2.56) has to be used in (3.2.59). Noting in this case that

$$\left. \begin{aligned}
 Q_0(y; \bar{y}) &= \frac{1}{2} \ln \left(\frac{\xi^2 + (y + \bar{y})^2}{\xi^2 + (y - \bar{y})^2} \right) \\
 \text{and} \\
 Q_1(y; \bar{y}) &= \left\{ \frac{y^2 + \bar{y}^2 + \xi^2}{4 y \bar{y}} \ln \left(\frac{\xi^2 + (y + \bar{y})^2}{\xi^2 + (y - \bar{y})^2} \right) - 1 \right\}
 \end{aligned} \right\} \quad (3.2.60)$$

and since the integral on the left-hand side can be explicitly done, we finally have

$$\begin{aligned}
 & y^3 + y^2 \left\{ [(1+\xi)^{1/3} - (1-\xi)^{1/3}] + \left(\frac{\xi^2 + (1+\xi)^{2/3} - y^2}{4y} \right) \ln \left(\frac{\xi^2 + (y + (1+\xi)^{1/3})^2}{\xi^2 + (y - (1+\xi)^{1/3})^2} \right) \right. \\
 & \quad \left. - \left(\frac{\xi^2 + (1-\xi)^{2/3} - y^2}{4y} \right) \ln \left(\frac{\xi^2 + (y + (1-\xi)^{1/3})^2}{\xi^2 + (y - (1-\xi)^{1/3})^2} \right) \right. \\
 & \quad \left. - \xi \left[\tan^{-1} \left(\frac{(1+\xi)^{1/3} + y}{\xi} \right) + \tan^{-1} \left(\frac{(1+\xi)^{1/3} - y}{\xi} \right) \right] \right. \\
 & \quad \left. + \xi \left[\tan^{-1} \left(\frac{(1-\xi)^{1/3} + y}{\xi} \right) + \tan^{-1} \left(\frac{(1-\xi)^{1/3} - y}{\xi} \right) \right] \right\} \bar{\Gamma}_{2 \uparrow 10}^{(1)}(y) \\
 & = \int d\bar{y} \left\{ \left(\frac{\xi^2 + y^2 + \bar{y}^2}{4} \right) \ln \left(\frac{\xi^2 + (y + \bar{y})^2}{\xi^2 + (y - \bar{y})^2} \right) - y \bar{y} \right\} (n_F(\omega_+(y)) - n_F(\omega_-(y))) \\
 & \quad \bar{\Gamma}_{2 \uparrow 10}^{(1)}(\bar{y}) \quad (3.2.61)
 \end{aligned}$$

Now note that if $\bar{\Gamma}_{2 \uparrow 10}^{(1)}(-y) = -\bar{\Gamma}_{2 \uparrow 10}^{(1)}(y)$, this equation still holds. The equation (3.2.61) is an inhomogeneous Fredholm equation of the second kind and hence admits of a power series solution. Furthermore, this has an iterative solution, the first iterate being the inhomogeneous part. Since the coefficient of $\bar{\Gamma}_{2 \uparrow 10}^{(1)}(y)$ in the left-hand side of (3.2.61) can be shown to be positive for positive y , it is clear that the solution $\bar{\Gamma}_{2 \uparrow 10}^{(1)}(y)$ has all

its terms negative. In view of the symmetry noted earlier, we may seek a power series solution in the form

$$\bar{\Gamma}_{2\uparrow 10}^{(1)}(y) = \sum_{n=0}^{\infty} a_{2n+1} y^{2n+1} \quad (3.2.62)$$

The integrations on the right-hand side can all be done in principle and thus a linear expression involving the coefficients $\{a_n\}$ is obtained. Equating the like powers of y on either side of this identity, we get a set of simultaneous linear inhomogeneous algebraic expressions for $\{a_n\}$, which can, therefore, be determined in principle. Once these coefficients are determined, $\bar{\Gamma}_{2\uparrow 10}^{(1)}$ is obtained and hence, $S(\xi, \zeta)$. In view of the cumbersome nature of this equation (3.2.61), we have, in the case of arbitrary magnetization, chosen a single term expansion in (3.2.62). Even this gives a very complicated expression for $S(\xi, \zeta)$. We here give S in the Coulomb and Stoner limits for the sake of simplicity:

$$\omega_{SW}^{SR} = \frac{q^2}{2m\xi} \left\{ 1 - \frac{1}{(K\theta^2/\epsilon_F)} \left[\frac{(1+\zeta)^{5/3} - (1-\zeta)^{5/3}}{5\xi} \right] \right\} \quad (3.2.63a)$$

where

$$\bar{\Gamma}_{2\uparrow 10}^{(1)}(y) = -\frac{3\xi^2}{4\xi} y \quad \text{for } \xi \rightarrow \infty.$$

and

$$\omega_{SW}^c = \frac{q^2}{2m\xi} \left\{ 1 - \frac{3}{10} \left(\frac{\pi}{ar_s} \right) \left[\frac{(1+\zeta)^{5/3} - (1-\zeta)^{5/3}}{(1+\zeta)^{1/3} - (1-\zeta)^{1/3}} \right] \right\} \quad (3.2.63b)$$

where

$$\bar{\Gamma}_{2\uparrow 10}^{(1)}(y) = -\frac{3}{2} \frac{y}{[(1+\zeta)^{1/3} - (1-\zeta)^{1/3}]} \quad \text{for } \xi = 0.$$

Note that (3.2.63a) is precisely the same as that obtained earlier by a rigorous method not involving the steps suggested above. In the paramagnetic limit, using the equilibrium $K\theta'/\epsilon_F$ and ar_s , respectively, it is found that the spin waves are unstable as must indeed be the case. Again for the F case, ($\xi=1$), ω_{SW} in both cases are positive when the corresponding equilibrium coupling strengths are used as they should be.

For the ferromagnetic case, however, we have carried out a three-term expansion in (3.2.62) and again a very cumbersome expression for $S(\xi)$ for all ξ 's obtained. For the sake of simplicity we again give the ~~Coulomb~~ ^{Stoner} and the Bloch limits only. In the Stoner case, a_3 and a_5 are identically zero to $[O(\xi^2)]$, as this is the only meaningful term here. In the Coulomb case, however, evaluating $(a_1 a_3 a_5)$ gives $S(\xi=0; \xi=1) = 0.3517$ and hence

$$\omega_{SW}^{c(\xi=1)} = q^2/2m \left(1 - \frac{5.344}{r_s} \right). \quad (3.2.64)$$

This must be compared with Herring's result

$$\omega_{SW}^{c(\xi=1)} = q^2/2m \left(1 - \frac{5.485}{r_s} \right).$$

Fukuda [12] gives 5.136 for this and this is wrong since he made an error in computing a_5 . It may be remarked that a two-term expansion gives 5.166 in agreement with Fukuda. It should now be stated that using Herring's spin-wave stability criterion using the equilibrium value $r_s = 5.45$ (Bloch[3]) we find that our calculation gives a positive ω_{SW} whereas Herring's gives an unstable spin wave (negative ω_{SW}). In view of this, we feel that our calculation is better than Herring's.

In the next section, the case of Bloch electrons will be dealt with in some detail.

3. The Case of Bloch Electrons

In Section 4 of Chapter II, suitable modifications for treating the single particle states in a periodic potential were outlined. In conjunction with (2.4.2), let us define the vertex parts in the Bloch scheme as follows:

$$\Gamma_i(l'l'k; q) = \int_{IBZ} b_{lk+q}^* \left(\frac{1}{2} \right) b_{l'k}(l') e^{iq \cdot 2} \Gamma_i(l'l'; 2) d^4 l d^4 l' d^4 2 \quad (3.3.1)$$

l : band index. Then the equations in the RPA including exchange can be written

$$\begin{aligned} \Gamma_i(l'l'k; q) = & -\tau_i \langle l'k+q | l'k \rangle - \\ & - i \sum_{l_1 l_2} \int \mathcal{V}_{l_1 q+\bar{q} l'k}^{lk+q l_2 \bar{q}} \left[\text{tr} \left\{ G_{l_1}(q+\bar{q}) \Gamma_i(l_1 l_2 \bar{q}; q) G_{l_2}(\bar{q}) \right\} \right] \frac{d^4 \bar{q}}{(2\pi)^4} + \\ & + i \sum_{l_1 l_2} \int \frac{d^4 \bar{q}}{(2\pi)^4} \mathcal{V}_{l'k l_1 q+\bar{q}}^{lk+q l_2 \bar{q}} G_{l_1}(q+\bar{q}) \Gamma_i(l_1 l_2 \bar{q}; q) G_{l_2}(\bar{q}) \end{aligned} \quad (3.3.2)$$

Here

$$\mathcal{V}_{l_3 k_3 l_4 k_4}^{l_1 k_1 l_2 k_2} = \int \int b_{l_1 k_1}^*(r_1) b_{l_2 k_2}^*(r_2) b_{l_3 k_3}(r_2) b_{l_4 k_4}(r_1) \mathcal{V}(r_1 - r_2) d^3 r_1 d^3 r_2 \quad (3.3.3)$$

Using the periodic properties of $b_{\underline{k}}$, it is seen that $\mathcal{V}^{\underline{l}_1 \underline{k}_1 \underline{l}_2 \underline{k}_2}_{\underline{l}_3 \underline{k}_3 \underline{l}_4 \underline{k}_4}$ is non-zero only if $\underline{k}_1 + \underline{k}_2 = \underline{k}_3 + \underline{k}_4 \pmod{\underline{K}}$ (\underline{K} : reciprocal lattice vector). Neglecting Umklapp processes (see Adler [46] for their effects) and using a Fourier representation for $\mathcal{V}(\underline{r}_1 - \underline{r}_2)$ one arrives at

$$\mathcal{V}^{\underline{l}_1 \underline{k}_1 \underline{l}_2 \underline{k}_2}_{\underline{l}_3 \underline{k}_3 \underline{l}_4 \underline{k}_4} = (2\pi)^3 \langle \underline{l}_1 \underline{k}_1 | \underline{l}_4 \underline{k}_4 \rangle \langle \underline{l}_2 \underline{k}_2 | \underline{l}_3 \underline{k}_3 \rangle \mathcal{V}(\underline{k}_1 - \underline{k}_4) \delta^{(3)}(\underline{k}_1 + \underline{k}_2 - \underline{k}_3 - \underline{k}_4) \quad (3.3.4)$$

Defining

$$\Gamma_i(\underline{l}' \underline{k}; \underline{q}) = \langle \underline{l}' \underline{k} + \underline{q} | \underline{l}' \underline{k} \rangle \Gamma_i'(\underline{l}' \underline{k}; \underline{q}) \quad (3.3.5)$$

and using (3.3.4) these equations can be recast into the form

$$\Gamma_i'(\underline{l}' \underline{k}; \underline{q}) = -\tau_i - \mathcal{V}(\underline{q}) \gamma_i^B(\underline{q}) + i \sum_{\underline{l}_1 \underline{l}_2} \int \frac{d^4 \underline{q}}{(2\pi)^4} \mathcal{V}(\underline{k} - \underline{q}) \mathcal{W}(\underline{l}' \underline{k} \underline{q}; \underline{l}_1 \underline{l}_2 \underline{q}) G_{\underline{l}_1}(\underline{q} + \underline{q}) \Gamma_i'(\underline{l}_1 \underline{l}_2 \underline{q}; \underline{q}) G_{\underline{l}_2}(\underline{q}) \quad (3.3.6)$$

where

$$\mathcal{W}(\underline{l}' \underline{k} \underline{q}; \underline{l}_1 \underline{l}_2 \underline{q}) = \frac{\langle \underline{l}' \underline{k} + \underline{q} | \underline{l}_1 \underline{q} + \underline{q} \rangle \langle \underline{l}_1 \underline{q} + \underline{q} | \underline{l}_2 \underline{q} \rangle \langle \underline{l}_2 \underline{q} | \underline{l}' \underline{k} \rangle}{\langle \underline{l}' \underline{k} + \underline{q} | \underline{l}' \underline{k} \rangle} \quad (3.3.7)$$

and

$$\gamma_i^B(\underline{q}) = i \sum_{\underline{l}_1 \underline{l}_2} \int \frac{d^4 \underline{q}}{(2\pi)^4} |\langle \underline{l}_1 \underline{q} + \underline{q} | \underline{l}_2 \underline{q} \rangle|^2 [\text{tr} \{ G_{\underline{l}_1}(\underline{q} + \underline{q}) \Gamma_i'(\underline{l}_1 \underline{l}_2 \underline{q}; \underline{q}) G_{\underline{l}_2}(\underline{q}) \}] \quad (3.3.8)$$

Assuming as before

$$\Gamma_i'(\mathcal{U}'k; q) = \Lambda_i(\mathcal{U}'k; q) + \mathcal{V}(q) \gamma_i^B(q) \Lambda_o(\mathcal{U}'k; q) \quad (3.3.9)$$

where

$$\Lambda_i(\mathcal{U}'k; q) = -\tau_i -$$

$$-i \sum_{\ell_1 \ell_2} \int \frac{d^4 \bar{q}}{(2\pi)^4} \mathcal{V}(k-\bar{q}) \mathcal{W}(\mathcal{U}'kq; \ell_1 \ell_2 \bar{q}) \cdot G_{\ell_1}(q+\bar{q}) \Lambda_i(\ell_1 \ell_2 \bar{q}; q) G_{\ell_2}(\bar{q}); \quad (3.3.10)$$

so that

$$\gamma_i^B(q) = \frac{i}{\mathcal{E}^B(q)} \sum_{\ell_1 \ell_2} \int \frac{d^4 \bar{q}}{(2\pi)^4} |<\ell_1 q+\bar{q} | \ell_2 \bar{q}>|^2 [\text{tr} \{G_{\ell_1}(q+\bar{q}) \Lambda_i(\ell_1 \ell_2 \bar{q}; q) G_{\ell_2}(\bar{q})\}] \quad (3.3.11)$$

with

$$\mathcal{E}^B(q) = 1 -$$

$$-i \mathcal{V}(q) \sum_{\ell_1 \ell_2} \int \frac{d^4 \bar{q}}{(2\pi)^4} |<\ell_1 q+\bar{q} | \ell_2 \bar{q}>|^2 [\text{tr} \{G_{\ell_1}(q+\bar{q}) \Lambda_o(\ell_1 \ell_2 \bar{q}; q) G_{\ell_2}(\bar{q})\}].$$

$$(3.3.12)$$

Finally

$$\begin{aligned}
\chi_{33}^B(q) = & i \sum_{l_1 l_2} \int \frac{d^4 \bar{q}}{(2\pi)^4} |< l_1 q + \bar{q} | l_2 \bar{q} >|^2 \\
& [\text{tr} \{ \tau_3 G_{l_1}(q+\bar{q}) \Lambda_3(l_1 l_2 \bar{q}; q) G_{l_2}(\bar{q}) \}] + \\
& + i \mathcal{V}(q) \gamma_3^B(q) \\
& \sum_{l_1 l_2} \int \frac{d^4 \bar{q}}{(2\pi)^4} |< l_1 q + \bar{q} | l_2 \bar{q} >|^2 [\text{tr} \{ \tau_3 G_{l_1}(q+\bar{q}) \Lambda_0(l_1 l_2 \bar{q}; q) G_{l_2}(\bar{q}) \}]
\end{aligned}
\tag{3.3.13}$$

and

$$\begin{aligned}
\chi_{+-}^B(q) = & i \sum_{l_1 l_2} \int \frac{d^4 \bar{q}}{(2\pi)^4} |< l_1 q + \bar{q} | l_2 \bar{q} >|^2 [\text{tr} \{ \tau^+ G_{l_1}(q+\bar{q}) \Lambda_2(l_1 l_2 \bar{q}; q) G_{l_2}(\bar{q}) \}] + \\
& + i \mathcal{V}(q) \gamma_1^B(q) \sum_{l_1 l_2} \int \frac{d^4 \bar{q}}{(2\pi)^4} |< l_1 q + \bar{q} | l_2 \bar{q} >|^2 [\text{tr} \{ \tau^+ G_{l_1}(q+\bar{q}) \Lambda_0(l_1 l_2 \bar{q}; q) G_{l_2}(\bar{q}) \}]
\end{aligned}
\tag{3.3.14}$$

In the 'plasma' RPA

$$\begin{aligned}
\varepsilon^B(q) = & 1 + \mathcal{V}(q) (A_I^B + B_I^B) = \\
= & 1 + i \mathcal{V}(q) \sum_{l_1 l_2} \int \frac{d^4 \bar{q}}{(2\pi)^4} |< l_1 q + \bar{q} | l_2 \bar{q} >|^2 [\text{tr} \{ G_{l_1}(q+\bar{q}) G_{l_2}(\bar{q}) \}]
\end{aligned}
\tag{3.3.15}$$

and similarly other expressions for χ_{33} , χ_{+-} , etc. One of the important features of the Bloch case is the appearance of additional sums on the band indices and the overlap integrals. The result for $\epsilon^B(q)$ in the unpolarized case is that first derived by Ehrenreich and Cohen [40] using the equation of motion method. These results here are generalized to include the polarizations. The above results are valid only when the local field corrections can be neglected since the Umklapp processes have been neglected entirely (Adler [44]). This neglect of local field corrections is justified when the bands are broad and far apart. In Appendix B the relation between these equations and those that can be derived by the equation of motion method will be given.

In view of the complexity of the results derived above, only the existence of spin waves will be discussed for the case of a single band, not overlapping with any others. As in Section 2 of this chapter, the equation describing the spin flip oscillation in the RPA including exchange is written in the form (3.2.42) for the F state (we have treated only F state here to keep the complications to a minimum):

$$\begin{aligned}
 (\omega - \epsilon_k(q)) \Gamma_{2\uparrow}(k; q) &= - \int \frac{d^3\bar{q}}{(2\pi)^3} \mathcal{V}(k-\bar{q}) \mathcal{W}(k\bar{q}; q) \Gamma_{2\uparrow}(\bar{q}; q) \\
 \epsilon_k(q) &= \epsilon(k+q) - \epsilon(k) - \int \frac{d^3\bar{q}}{(2\pi)^3} |\langle k | \bar{q} \rangle|^2 \mathcal{V}(k-\bar{q})
 \end{aligned} \tag{3.3.16}$$

where $\epsilon(k)$ is the band energy.

In the almost free electron limit, $\langle k|q \rangle \sim 1$, and so $\omega \sim 1$; since $\mathcal{V}(k) = 4\pi e^2/k^2$ the arguments of the previous section, case (C), go through and hence spin waves exist in this case.

In the tight binding limit, where the overlap integrals can be expressed in terms of Wannier orbitals, $a(\underline{r} - \underline{l})$, \underline{l} is the lattice site, and if both \underline{k} and \underline{q} are near zero,

$$\begin{aligned} \langle k | \bar{q} \rangle &= \int_{\text{unit cell}} u_k^*(\underline{r}) u_{\bar{q}}(\underline{r}) d^3r \\ &= \sum_{\underline{l}_1 \underline{l}_2} e^{-i(\underline{k} \cdot \underline{l}_1 - \bar{\underline{q}} \cdot \underline{l}_2)} \int_{\text{unit cell}} a^*(\underline{r} - \underline{l}_1) a(\underline{r} - \underline{l}_2) d^3r \end{aligned}$$

The integral

$$\int_{\text{unit cell}} a^*(\underline{r} - \underline{l}_1) a(\underline{r} - \underline{l}_2) d^3r$$

is the overlap between two Wannier states, $I_{11'}$. In the extreme tight binding limit, $I_{11'} \sim I_1 \delta_{11'}$, and if \underline{k} and \underline{k}' are ~ 0 , $\sum_{\underline{l}} \rightarrow \int d^3l$ so that $\langle k | \bar{q} \rangle = O(|k - \bar{q}|)$. The arguments of Section 2, case (C) of this chapter are applicable so that the spin waves are seen to exist in this case also, since $\omega(k\bar{q}q) \sim O^2(|k - \bar{q}|)$ and the equation for ω is

$$(\omega - \epsilon_k(q)) \Gamma_{2\uparrow\uparrow}(k; q) = - \int \frac{d^3\bar{q}}{(2\pi)^3} \mathcal{V}(k - \bar{q}) O^2(|k - \bar{q}|) \Gamma_{2\uparrow\uparrow}(\bar{q}; q)$$

with

$$\epsilon_k(q) = \epsilon(k+q) - \epsilon(k) - \int \frac{d^3\bar{q}}{(2\pi)^3} \mathcal{V}(k-\bar{q}) O^2(|k-\bar{q}|).$$

There is another approximation to the integral (3.3.4) suggested by Antonoff [29]. The corresponding results are here derived using the present technique, since they follow quite easily from the expressions already derived. Antonoff makes the "degenerate kernel" approximation which consists in taking, in the single band scheme

$$\mathcal{V}_{k_3 k_4}^{k_1 k_2} \approx \mathcal{V}_c(k_1 - k_4) + \mathcal{V}_{ex}(k_1 - k_3). \quad (3.3.17)$$

What is done here is to write $\mathcal{V}_{k_3 k_4}^{k_1 k_2}$ in terms of Wannier orbitals, and in the resulting expression retain only two-center integrals. Then (3.3.2) takes the form (in the one-band case)

$$\begin{aligned} \Gamma_i(k; q) = & -\tau_i - i \int \frac{d^4\bar{q}}{(2\pi)^4} (\mathcal{V}_c(q) + \mathcal{V}_{ex}(k-\bar{q})) \\ & [\text{tr} \{ G(q+\bar{q}) \Gamma_i(\bar{q}; q) G(\bar{q}) \}] + \\ & + i \int \frac{d^4\bar{q}}{(2\pi)^4} (\mathcal{V}_c(k-\bar{q}) + \mathcal{V}_{ex}(q)) G(q+\bar{q}) \Gamma_i(\bar{q}; q) G(\bar{q}) \end{aligned} \quad (3.3.18)$$

In this one further neglects $\mathcal{V}_{ex}(k-\bar{q})$ in the second term and $\mathcal{V}_c(k-\bar{q})$ in the third. Then a calculation similar to case (B) of the present chapter follows:

$$\gamma_0^{\text{III}}(q) = \frac{-(A_{\text{III}} + B_{\text{III}} - 2\mathcal{V}_{\text{ex}}(q)A_{\text{III}}B_{\text{III}})}{[1-(\mathcal{V}_{\text{ex}}(q)-\mathcal{V}_{\text{c}}(q))(A_{\text{III}}+B_{\text{III}})+\mathcal{V}_{\text{ex}}(q)(\mathcal{V}_{\text{ex}}(q)-2\mathcal{V}_{\text{c}}(q))A_{\text{III}}B_{\text{III}}]} \quad (3.3.19)$$

$$\gamma_1^{\text{III}}(q) = 0 \quad (3.3.20)$$

$$\gamma_2^{\text{III}}(q) = 0 \quad (3.3.21)$$

$$\gamma_3^{\text{III}}(q) = \frac{-(A_{\text{III}} - B_{\text{III}})}{[1-(\mathcal{V}_{\text{ex}}(q)-\mathcal{V}_{\text{c}}(q))(A_{\text{III}}+B_{\text{III}})+\mathcal{V}_{\text{ex}}(q)(\mathcal{V}_{\text{ex}}(q)-2\mathcal{V}_{\text{c}}(q))A_{\text{III}}B_{\text{III}}]} \quad (3.3.22)$$

$$\chi_{33}^{\text{III}}(q) = \frac{-(A_{\text{III}} + B_{\text{III}} - 2(\mathcal{V}_{\text{ex}}(q) - 2\mathcal{V}_{\text{c}}(q))A_{\text{III}}B_{\text{III}})}{[1-(\mathcal{V}_{\text{ex}}(q)-\mathcal{V}_{\text{c}}(q))(A_{\text{III}}+B_{\text{III}})+\mathcal{V}_{\text{ex}}(q)(\mathcal{V}_{\text{ex}}(q)-2\mathcal{V}_{\text{c}}(q))A_{\text{III}}B_{\text{III}}]} \quad (3.3.23)$$

$$\chi_{+-}^{\text{III}}(q) = \frac{-C_{\text{III}}}{(1-\overline{\mathcal{V}}_{\text{ex}}C_{\text{III}})} \quad (3.3.24)$$

$$\omega_{\pm}^{\text{III}}(q) = \epsilon(q) - \frac{1}{2} \int \frac{d^3\bar{q}}{(2\pi)^3} (\mathcal{V}_{\text{c}}(q-\bar{q}) + \mathcal{V}_{\text{ex}}(0)) n(\bar{q}) \mp$$

$$\mp \frac{1}{2} \int \frac{d^3\bar{q}}{(2\pi)^3} (\mathcal{V}_{\text{c}}(q-\bar{q}) + \mathcal{V}_{\text{ex}}(0)) \sigma_3(\bar{q}) \quad (3.3.25)$$

In (3.3.25) $\mathcal{V}_{\text{c}}(q-\bar{q})$ is also neglected. In the unpolarized case one obtains

$$\gamma_0^{III} = -2A_{III}/(1 + (2v_c(q) - v_{ex}(q))A_{III}) \quad (3.3.26)$$

$$\gamma_1^{III} = \gamma_2^{III} = \gamma_3^{III} = 0 \quad (3.3.27)$$

$$\chi_{33}^{III} = -2A_{III}/(1 - v_{ex}(q)A_{III}) = 2\chi_{+-}^{III} \quad (3.3.28)$$

From these results one may notice the following features, even though many terms are neglected in arriving at these results. The Coulomb and the exchange integrals appear in all the correlation functions except χ_{+-}^{III} where only v_{ex} appears. This is significant, and the reason why in the "plasma" RPA χ_{+-} did not show the pole structure directly and why it did in case (B) now appears obvious, even though this fact that exchange has to be taken into account fully was stressed earlier. In case (B), however, we had taken $v_{ex} = v_c = \bar{v}$, which when substituted in the above set of expressions give back those found already. The results of case (A) follow if v_{ex} is neglected altogether.

It must be mentioned here that if the "degenerate kernel" approximation is made in the Hamiltonian itself after rewriting it in the Bloch representation:

$$H = \sum_{k\sigma} \epsilon(k) a_{k\sigma}^\dagger a_{k\sigma} + \frac{1}{2} \sum_{k_1 k_2} \sum_{k_3 k_4} \sum_{\sigma_1 \sigma_2} v_{k_3 k_4}^{k_1 k_2} a_{k_1 \sigma_1}^\dagger a_{k_2 \sigma_2}^\dagger a_{k_3 \sigma_2} a_{k_4 \sigma_1} \quad (3.3.29)$$

($k_1 + k_2 = k_3 + k_4$)

one may then combine the terms in such a way as to get an explicit Heisenberg-type interaction. Actually, $\mathcal{V}_{\text{ex}}(q)$ goes here with terms which can be cast into the form $\underline{g}(q)$. $\underline{g}(-q)$ which is just the Heisenberg result. Now if RPA is used for constructing the various correlation functions, the results obtained here are recovered. This has been verified by the author. Antonoff [29] in his thesis neglected $\mathcal{V}_c(q)$ entirely and obtained spin waves. As remarked above, this is equivalent to assuming a Heisenberg interaction between spins. In later work with F. Englert [29] Antonoff has included $\mathcal{V}_c(q)$ and obtained the results given above. They used an equation of motion method.

In summary, the possibility of spin-wave excitations in an itinerant model is here shown under various model interactions within the context of RPA. Moreover, the case of an electron gas interacting with a Yukawa potential is studied explicitly and the coefficient of q^2 in the ferromagnetic state is determined. The results are in good agreement with those obtained by Herring [22, 23] in the appropriate limits. The collective excitations for the Overhauser situation are not examined here.

There are many objections to the use of Yukawa potential (even though potentials of this type with Thomas-Fermi screening are suggestive) in such calculations as are undertaken in the present work. The first major objection is that it is an arbitrary choice and in reality the situation may be more complex. Secondly, even if the choice be arbitrary, no method is here outlined to determine the screening parameter from first principles. Thirdly, the screening of the interaction in this way is known to reduce the contribution of the exchange energy to the cohesive energy enormously if the screening radii are chosen to give agreement with the observed specific heat ($\xi k_F \sim 10^8 \text{ cm}^{-1}$). (See Pines [38].) In spite of these objections the effect of screening on the various properties of the electron gas is most easily investigated analytically, by using a Yukawa potential.

There are several possible directions of extension of the present work. Concrete results are derived only for $T = 0^\circ \text{K}$. These must be generalized to finite temperatures. This extension should settle the query whether the low temperature magnetization is the Bloch $T^{3/2}$ or the Stoner T^2 . It is almost clear from the present work, that at very low temperatures one must have $T^{3/2}$ behavior. This view has been put forward by Brooks [6b] and very recently by Mattis [47] also. There have been some diagrammatic analyses of this problem which are not quite rigorous or conclusive. The equations describing the magnetization are quite nonlinear. Some self-consistent way of calculating the magnetization at low temperatures must be

developed as was stressed at the end of the last chapter. The notion often expressed and notably by Edwards [25] that the Stoner and Bloch terms for magnetization and specific heat will both be present is almost certainly wrong, as the existence of q_{\max} for spin waves clearly indicates. Even at $T = 0^\circ\text{K}$, the problem has to be done more completely by including all the possible processes in computing the ground-state energy of the system as a function of magnetization. The present work indicates very clearly that a mere comparison of \bar{F} and \bar{P} state energies is certainly not sufficient to determine the nature of the ground state, as was done by Cooper [13] and Shimizu [11]. This is hard only in the sense of numerical analysis but the way it can be handled is outlined in this work, for the expression for the dielectric constant is here derived from which the ground-state energy can be computed as was done by Cooper. The third extension, which is not considered here at all, is the collective excitations of the system when Overhauser type ground states exist. These must show some new characteristics. Professor P. C. Martin considers SDW as an itinerant version of the usual antiferromagnetism. If so, one may expect antiferromagnetic spin-wave type oscillations in the SDW case. We have now succeeded in solving this problem in an approximate way, and the results on this and other matters concerning itinerant antiferromagnetism will be dealt with in a separate technical report. The fourth extension is a more thorough investigation of

the results given here for Bloch electrons. The fifth problem is the examination of the Overhauser problem once again in the Bloch scheme. The investigation of SDW for Bloch waves must be of interest in real solids as extrapolation from the free gas results to the real cases is often misleading. The outstanding problem of all, of course, is a complete investigation, even within HF, of all the possible ground states including those of broken symmetry. The phase diagrams given in Figs. 2a, b do not include the superconducting and the SDW ground states and if these could be somehow incorporated in this plot one would have a more complete account of the electron gas, even at $T = 0^\circ\text{K}$.

APPENDIX A

SPECTRAL REPRESENTATION OF THE CORRELATION FUNCTIONS

By virtue of the definition, commutation rules, the Hermiticity condition, and the trace structure of the correlation functions defined by (3.1.2), a set of formal relations is obtained for their spectral weight functions. These are given here without derivation (c.f. Chapter II, section 1).

$A_{\rho\rho}(r_1 r_2; \omega)$, $A_{33}(r_1 r_2; \omega)$ and $A_{+-}(r_1 r_2; \omega)$ correspond to γ_0 , χ_{33} , and χ_{+-} .

$$A_{\rho\rho}^*(r_1 r_2; \omega) = A_{\rho\rho}(r_2 r_1; -\omega)$$

$$\int \frac{d\omega}{2\pi} A_{\rho\rho}(r_1 r_2; \omega) = 0$$

$$A_{\rho\rho}(r_1 r_2; \omega) = i \lim_{\epsilon \rightarrow 0} [\gamma_0(r_1 r_2; \omega + i\epsilon) - \gamma_0(r_1 r_2; \omega - i\epsilon)]$$

$$\langle \rho(2) \rho(1) \rangle \big|_{t_2=t_1^+} = \int \frac{d\omega}{2\pi} \frac{A_{\rho\rho}(r_1 r_2; \omega)}{(e^{\beta\omega} - 1)}$$

and

$$\gamma_0(12; z) = \int \frac{d\bar{\omega}}{2\pi i} \frac{A_{\rho\rho}(r_1 r_2; \bar{\omega})}{\bar{\omega} - z} \quad (\text{A-1})$$

(z is a complex variable)

$$A_{33}^*(\underline{r}_1 \underline{r}_2; \omega) = A_{33}(\underline{r}_2 \underline{r}_1; -\omega)$$

$$\int \frac{d\omega}{2\pi} A_{33}(\underline{r}_1 \underline{r}_2; \omega) = 0$$

$$A_{33}(\underline{r}_1 \underline{r}_2; \omega) = i \lim_{\epsilon \rightarrow 0} [\chi_{33}(\underline{r}_1 \underline{r}_2; \omega + i\epsilon) - \chi_{33}(\underline{r}_1 \underline{r}_2; \omega - i\epsilon)]$$

$$\langle \hat{\sigma}_3(2) \hat{\sigma}_3(1) \rangle |_{t_2=t_1+} = \int \frac{d\omega}{2\pi} \frac{A_{33}(\underline{r}_1 \underline{r}_2; \omega)}{(e^{\beta\omega} - 1)}$$

and

$$\chi_{33}(12; z) = \int \frac{d\bar{\omega}}{2\pi i} \frac{A_{33}(\underline{r}_1 \underline{r}_2; \bar{\omega})}{\bar{\omega} - z} \quad (A-2)$$

$$A_{+-}^*(\underline{r}_1 \underline{r}_2; \omega) = A_{-+}(\underline{r}_2 \underline{r}_1; -\omega)$$

$$\int \frac{d\omega}{2\pi} A_{+-}(\underline{r}_1 \underline{r}_2; \omega) = \langle \sigma_3(\underline{r}_1) \rangle \delta^{(3)}(\underline{r}_1 - \underline{r}_2)$$

(equal time commutation rule)

$$[\sigma_+(1), \sigma_-(2)]_- = \sigma_3(1) \delta^{(3)}(\underline{r}_1 - \underline{r}_2)$$

$$A_{+-}(\underline{r}_1 \underline{r}_2; \omega) = i \lim_{\epsilon \rightarrow 0} [\chi_{+-}(\underline{r}_1 \underline{r}_2; \omega + i\epsilon) - \chi_{+-}(\underline{r}_1 \underline{r}_2; \omega - i\epsilon)]$$

$$\langle \hat{\sigma}_+(2) \hat{\sigma}_-(1) \rangle |_{t_2=t_1+} = \int \frac{d\omega}{2\pi} \frac{A_{+-}(\underline{r}_1 \underline{r}_2; \omega)}{(e^{\beta\omega} - 1)}$$

and

$$\chi_{+-}(12; z) = \int \frac{d\bar{\omega}}{2\pi i} \frac{A_{+-}(\underline{r}_1 \underline{r}_2; \bar{\omega})}{\bar{\omega} - z} \quad (A-3)$$

THE RELATION BETWEEN THE EQUATION OF MOTION METHOD AND THE GREEN'S FUNCTION METHOD

Here the equations describing the various collective excitations given in Chapter III, will be rederived by extending the equation of motion method to the polarized medium for Bloch electrons. Incidentally, this extends Wolff's [31] method to Bloch electrons and also includes the free electron result as a special case. The Hamiltonian is written in the Bloch representation:

$$\begin{aligned}
 H = & \sum_{\ell_1 k_1} \sum_{\sigma_1} \epsilon_{\ell_1}(k_1) a_{k_1 \ell_1 \sigma_1}^\dagger a_{k_1 \ell_1 \sigma_1} + \\
 & + \frac{1}{2} \sum_{\ell_1 k_1} \sum_{\ell_2 k_2} \sum_{\ell_3 k_3} \sum_{\ell_4 k_4} \sum_{\sigma_1 \sigma_2} v_{k_1 \ell_1 k_2 \ell_2}^{\ell_3 \ell_4} a_{k_1 \ell_1 \sigma_1}^\dagger a_{k_2 \ell_2 \sigma_2}^\dagger a_{k_3 \ell_3 \sigma_2} a_{k_4 \ell_4 \sigma_1} + \\
 & \quad (k_1 + k_2 = k_3 + k_4 \pmod{K}) \\
 & + \sum_{\ell_1 \ell_2} \sum_{q_1 k_2} \langle k_2 \ell_1 | k_2 + q_1 \ell_2 \rangle \left\{ a_{k_2 \ell_1}^\dagger a_{k_2 + q_1 \ell_2}^\dagger U_+(q_1) + \right. \\
 & + a_{k_2 \ell_1}^\dagger a_{k_2 + q_1 \ell_2} U_-(q_1) + (a_{k_2 \ell_1}^\dagger a_{k_2 + q_1 \ell_2} + a_{k_2 \ell_1} a_{k_2 + q_1 \ell_2}^\dagger) U_0(q_1) + \\
 & \left. + (a_{k_2 \ell_1}^\dagger a_{k_2 + q_1 \ell_2} - a_{k_2 \ell_1} a_{k_2 + q_1 \ell_2}^\dagger) U_3(q_1) \right\}. \tag{B-1}
 \end{aligned}$$

a^\dagger and a are the creation, annihilation operators for Bloch electrons satisfying the usual anticommutation rules. Then the equations of motion in the RPA for various operators are constructed, after using

$$\mathcal{V}_{k_3 \ell_3 k_4 \ell_4}^{k_1 \ell_1 k_2 \ell_2} = (2\pi)^3 \delta^{(3)}(k_1 + k_2 - k_3 - k_4) \mathcal{V}(k_1 - k_4)$$

$$\langle k_1 \ell_1 | k_4 \ell_4 \rangle \langle k_2 \ell_2 | k_3 \ell_3 \rangle.$$

(Umklapp processes are neglected as in the text)

$$\Gamma^{\sigma\sigma'}(k\ell\ell'; q) = \langle a_{k\ell'\sigma}^\dagger a_{k+q\ell\sigma'} \rangle \sim e^{-i\omega t} \quad (B-2)$$

$$\begin{aligned} & [\omega - \omega_{\ell'}^+(k+q) + \omega_{\ell'}^+(k)] \Gamma^{\uparrow\uparrow}(k\ell\ell'; q) = \\ & = [n_F(\omega_{\ell'}^+(k+q)) - n_F(\omega_{\ell'}^+(k))] \langle k+q\ell | k\ell' \rangle \left\{ -U_0(q) - U_3(q) - \right. \\ & \quad - \mathcal{V}(q) \sum_{q'} \sum_{\ell_1 \ell_2} \sum_{\sigma} \langle q'\ell_2 | q'+q\ell_1 \rangle \Gamma^{\sigma\sigma}(q'\ell_1 \ell_2; q) + \\ & \quad \left. + \sum_{q'} \sum_{\ell_1 \ell_2} \frac{\mathcal{V}(k-q') \mathcal{V}(k\ell\ell'q; q'\ell_1 \ell_2)}{\langle q'+q\ell_1 | q'\ell_2 \rangle} \Gamma^{\uparrow\uparrow}(q'\ell_1 \ell_2; q) \right\} \quad (B-3) \end{aligned}$$

\mathcal{V} is as defined in (3.3.7)

$$\begin{aligned} & [\omega - \omega_{\ell'}^-(k+q) + \omega_{\ell'}^-(k)] \Gamma^{\downarrow\downarrow}(k\ell\ell'; q) = \\ & = [n_F(\omega_{\ell'}^-(k+q)) - n_F(\omega_{\ell'}^-(k))] \langle k+q\ell | k\ell' \rangle \left\{ -U_0(q) + U_3(q) - \right. \\ & \quad - \mathcal{V}(q) \sum_{q'} \sum_{\ell_1 \ell_2} \sum_{\sigma} \langle q'\ell_2 | q'+q\ell_1 \rangle \Gamma^{\sigma\sigma}(q'\ell_1 \ell_2; q) + \\ & \quad \left. + \sum_{q'} \sum_{\ell_1 \ell_2} \frac{\mathcal{V}(k-q') \mathcal{V}(k\ell\ell'q; q'\ell_1 \ell_2)}{\langle q'+q\ell_1 | q'\ell_2 \rangle} \Gamma^{\downarrow\downarrow}(q'\ell_1 \ell_2; q) \right\} \quad (B-4) \end{aligned}$$

and

$$\begin{aligned}
 & (\omega - \omega_{\ell}^{-}(k+q) + \omega_{\ell'}^{+}(k)) \Gamma_{\ell\ell'}^{\dagger\dagger}(k\ell\ell'; q) = \\
 & = [n_F(\omega_{\ell}^{-}(k+q)) - n_F(\omega_{\ell'}^{+}(k))] \langle k+q\ell | k\ell' \rangle \left\{ -U_1(q) + \right. \\
 & \left. + \sum_{q'} \sum_{\ell_1\ell_2} \frac{\mathcal{V}(k-q') \mathcal{V}(k\ell\ell'q; q'\ell_1\ell_2)}{\langle q'+q\ell_1 | q'\ell_2 \rangle} \Gamma_{\ell_1\ell_2}^{\dagger\dagger}(q'\ell_1\ell_2; q) \right\} \quad (B-5)
 \end{aligned}$$

with

$$\omega_{\ell}^{\pm}(k) = \epsilon_{\ell}(k) - \frac{1}{2} \sum_{q'\ell'} |\langle q'\ell' | k\ell \rangle|^2 \mathcal{V}(k-q') (n_{\ell'}(q') \pm \sigma_{3\ell'}(q')). \quad (B-6)$$

To see the connection with the vertex part equations, namely (3.3.6), one first notices that the right side of (3.3.6) is independent of the frequency part of k , the first index of the vertex function, so that one may assert that the solution of this equation is of the form

$$\Gamma_{\ell\ell'}^{\dagger\dagger}(k\ell\ell'; q) = \Gamma_{\ell\ell'}^{\dagger\dagger}(\underline{k}\ell\ell'; q).$$

Then the $\bar{\omega}$ integrations can be carried out in the right-hand side and assuming the G 's to be diagonal, one gets, writing it in the component form:

$$\begin{aligned}
(\Gamma_i'(\underline{k}\ell\ell'; q\omega))_{\sigma\sigma'} &= (\tau_i)_{\sigma\sigma'} - \\
&- \delta_{\sigma\sigma'} \mathcal{V}(q) \sum_{q'} \sum_{\ell_1 \ell_2} \sum_{\sigma} \left(\frac{n_F(\omega_{\ell_1}^{\sigma}(q+q')) - n_F(\omega_{\ell_2}^{\sigma}(q'))}{\omega - \omega_{\ell_1}^{\sigma}(q+q') + \omega_{\ell_2}^{\sigma}(q')} \right) \\
&\quad | \langle q'+q\ell_1 | q'\ell_2 \rangle |^2 (\Gamma_i'(\underline{q}'\ell_1\ell_2; q\omega))_{\sigma\sigma'} + \\
&+ \sum_{q'} \sum_{\ell_1 \ell_2} \mathcal{V}(k-q') \mathcal{W}(k\ell\ell'q; q'\ell_1\ell_2) \\
&\quad \left(\frac{n_F(\omega_{\ell_1}^{\sigma}(q+q')) - n_F(\omega_{\ell_2}^{\sigma}(q'))}{\omega - \omega_{\ell_1}^{\sigma}(q+q') + \omega_{\ell_2}^{\sigma}(q')} \right) (\Gamma_i'(\underline{q}'\ell_1\ell_2; q))_{\sigma\sigma'} \quad (B-7)
\end{aligned}$$

Now let

$$(\Gamma_i'(\underline{k}\ell\ell'; q\omega))_{\sigma\sigma'} = \left(\frac{\omega - \omega_{\ell}^{\sigma}(k+q) + \omega_{\ell'}^{\sigma'}(k)}{n_F(\omega_{\ell}^{\sigma}(k+q)) - n_F(\omega_{\ell'}^{\sigma'}(k))} \right) \frac{\Gamma_i^{\sigma\sigma'}(\underline{k}\ell\ell'; q)}{\langle k+q\ell | k\ell' \rangle} \quad (B-8)$$

then

$$\begin{aligned}
&(\omega - \omega_{\ell}^{\sigma}(k+q) + \omega_{\ell'}^{\sigma'}(k)) \Gamma_i^{\sigma\sigma'}(\underline{k}\ell\ell'; q) = \\
&= [n_F(\omega_{\ell}^{\sigma}(k+q)) - n_F(\omega_{\ell'}^{\sigma'}(k))] \langle k+q\ell | k\ell' \rangle \left\{ -(\tau_i)_{\sigma\sigma'} - \right. \\
&- \delta_{\sigma\sigma'} \mathcal{V}(q) \sum_{q'} \sum_{\ell_1 \ell_2} \sum_{\sigma} (\langle q'\ell_2 | q'+q\ell_1 \rangle) \Gamma_i^{\sigma\sigma'}(q'\ell_1\ell_2; q) + \\
&+ \sum_{q'} \sum_{\ell_1 \ell_2} \frac{\mathcal{V}(k-q') \mathcal{W}(k\ell\ell'q; q'\ell_1\ell_2)}{\langle q'+q\ell_1 | q'\ell_2 \rangle} \Gamma_i^{\sigma\sigma'}(q'\ell_1\ell_2; q) \left. \right\} \quad (B-9)
\end{aligned}$$

which are identical in structure with those derived above (B - 3, 4, 5) except for the external field terms which have been swallowed in the Green's function technique as the vertex part involves a variational derivative with respect to these and, hence, their presence here appears as $(\tau_i)_{\sigma\sigma'}$. (The notation used here is very slightly different from the text and should cause no great confusion.)

OVERHAUSER SOLUTIONS INVOLVING BLOCH ELECTRONS

In the Epilogue, the fifth problem mentioned concerns the extension of the results of Overhauser [18] obtained in Section II-3 to Bloch electrons. This is particularly of use since the Chromium-Rhenium system seems to show an SDW character demanding a two-band model. This was brought to the attention of one of us (A. K. Rajagopal) by Dr. Van Zandt of Lincoln Laboratories. In this appendix we give a generalization of our results of the Stoner theory for Bloch electrons given in Section II-4 so as to give an Overhauser-type theory for Bloch electrons. The results of Section II-4 follow when $Q = 0$ and those of Section II-3 follow when the Bloch functions are replaced by plane waves, and the band indices omitted. The results obtained here are all formal.

In order to arrive at a suitable generalization, we assume that the electron of spin up and wave vector k in band l is associated only with the one of spin down in the same band but with a vector $(k+Q)$. With this prescription, the following redefinitions of the expression (2.3.1) are made:

$$\begin{aligned}
 G_{\uparrow\uparrow}(11') &= \sum_{l'} \int_{IBZ} \frac{d^3 k'}{(2\pi)^3} b_{l'k'}^{(1)} b_{l'k'}^{*(1')} G_{\uparrow\uparrow}(l'k'; t_1 - t_{1'}) \\
 G_{\downarrow\downarrow}(11') &= \sum_{l'} \int_{IBZ} \frac{d^3 k'}{(2\pi)^3} b_{l'k'+Q}^{(1)} b_{l'k'+Q}^{*(1')} G_{\downarrow\downarrow}(l'k'; t_1 - t_{1'}) \\
 G_{\uparrow\downarrow}(11') &= \sum_{l'} \int_{IBZ} \frac{d^3 k'}{(2\pi)^3} b_{l'k'}^{(1)} b_{l'k'+Q}^{*(1')} G_{\uparrow\downarrow}(l'k'; t_1 - t_{1'}) \\
 G_{\downarrow\uparrow}(11') &= \sum_{l'} \int_{IBZ} \frac{d^3 k'}{(2\pi)^3} b_{l'k'+Q}^{(1)} b_{l'k'}^{*(1')} G_{\downarrow\uparrow}(l'k'; t_1 - t_{1'})
 \end{aligned}
 \tag{C-1}$$

C-1

Then a calculation similar to the one given in Section II-3 follows and we give here only the final results.

$$\left. \begin{aligned}
 \epsilon_{l\uparrow}(k) &= \epsilon_l(k) + i \sum_{l'} \int_{\text{IBZ}} \mathcal{V}_{lk, l'k'}^{lk, l'k'} G_{l\uparrow}^{<}(l'k'; \omega') e^{i\omega'0^+} \frac{d^3 k' d\omega'}{(2\pi)^4} \\
 \epsilon_{l\downarrow}(k) &= \epsilon_l(k+Q) + i \sum_{l'} \int_{\text{IBZ}} \mathcal{V}_{lk+Q, l'k'+Q}^{lk+Q, l'k'+Q} G_{l\downarrow}^{<}(l'k'; \omega') e^{i\omega'0^+} \frac{d^3 k' d\omega'}{(2\pi)^4} \\
 g_{l\uparrow}(lk) &= i \sum_{l'} \int_{\text{IBZ}} \mathcal{V}_{lk, l'k'+Q}^{lk, l'k'+Q} G_{l\uparrow}^{<}(l'k'; \omega') e^{i\omega'0^+} \frac{d^3 k' d\omega'}{(2\pi)^4} \\
 g_{l\downarrow}(lk) &= i \sum_{l'} \int_{\text{IBZ}} \mathcal{V}_{lk+Q, l'k'}^{lk+Q, l'k'} G_{l\downarrow}^{<}(l'k'; \omega') e^{i\omega'0^+} \frac{d^3 k' d\omega'}{(2\pi)^4}
 \end{aligned} \right\} \quad (\text{C-2})$$

Here $\epsilon_l(k)$ is the energy of the electron in band l , and the IBZ indicates that the integration in k space is confined to the first Brillouin zone. As in Section II-4,

$$\mathcal{V}_{l_1 k_1, l_2 k_2}^{l_3 k_3, l_4 k_4} = \int \int b_{l_1 k_1}^* (1) b_{l_2 k_2}^* (2) \mathcal{V}^{(1-2)} b_{l_3 k_3} (2) b_{l_4 k_4} (1) d^3 1 d^3 2$$

Moreover,

$$\omega_l^{\pm}(k) = \left(\frac{\epsilon_{l\uparrow}(k) + \epsilon_{l\downarrow}(k)}{2} \right) \pm \sqrt{\left(\frac{\epsilon_{l\uparrow}(k) - \epsilon_{l\downarrow}(k)}{2} \right)^2 + g_{l\uparrow}(lk) g_{l\downarrow}(lk)} \quad (\text{C-3})$$

Thus, in Section II-3 we may replace $\theta_{\underline{k}}$ by $\theta_{\underline{l}\underline{k}}$ so that one has finally

$$G(\underline{l}\underline{k}; \omega) =$$

$$= \begin{pmatrix} [\cos^2 \theta_{\underline{l}\underline{k}} g_+(\underline{l}\underline{k}; \omega) + \sin^2 \theta_{\underline{l}\underline{k}} g_-(\underline{l}\underline{k}; \omega)] & \cos \theta_{\underline{l}\underline{k}} \sin \theta_{\underline{l}\underline{k}} \sqrt{\frac{g_{\uparrow\uparrow}(\underline{l}\underline{k})}{g_{\uparrow\uparrow}(\underline{l}\underline{k})}} [g_+(\underline{l}\underline{k}; \omega) - g_-(\underline{l}\underline{k}; \omega)] \\ [\cos \theta_{\underline{l}\underline{k}} \sin \theta_{\underline{l}\underline{k}} \sqrt{\frac{g_{\uparrow\uparrow}(\underline{l}\underline{k})}{g_{\uparrow\uparrow}(\underline{l}\underline{k})}} [g_+(\underline{l}\underline{k}; \omega) - g_-(\underline{l}\underline{k}; \omega)] & [\sin^2 \theta_{\underline{l}\underline{k}} g_+(\underline{l}\underline{k}; \omega) + \cos^2 \theta_{\underline{l}\underline{k}} g_-(\underline{l}\underline{k}; \omega)] \end{pmatrix} \quad (C-4)$$

where

$$g_{\pm}(\underline{l}\underline{k}; \omega) = 1/[\omega - \omega_{\underline{l}}^{\pm}(\underline{k})]. \quad (C-5)$$

Finally then

$$\begin{aligned} \epsilon_{\uparrow\uparrow}(\underline{k}) &= \epsilon_{\uparrow}(\underline{k}) - \sum_{\underline{l}'} \int_{\text{IBZ}} \frac{d^3 k'}{(2\pi)^3} \mathcal{V}_{\underline{l}\underline{k} \underline{l}' \underline{k}'}^{\underline{l}\underline{k} \underline{l}' \underline{k}'} [\cos^2 \theta_{\underline{l}' \underline{k}', n_F(\omega_{\underline{l}'}^+(\underline{k}')) + \sin^2 \theta_{\underline{l}' \underline{k}', n_F(\omega_{\underline{l}'}^-(\underline{k}'))}] \\ \epsilon_{\uparrow\downarrow}(\underline{k}) &= \epsilon_{\uparrow}(\underline{k} + \underline{Q}) - \sum_{\underline{l}'} \int_{\text{IBZ}} \frac{d^3 k'}{(2\pi)^3} \mathcal{V}_{\underline{l}\underline{k} + \underline{Q} \underline{l}' \underline{k}' + \underline{Q}}^{\underline{l}\underline{k} + \underline{Q} \underline{l}' \underline{k}' + \underline{Q}} [\sin^2 \theta_{\underline{l}' \underline{k}', n_F(\omega_{\underline{l}'}^+(\underline{k}')) + \cos^2 \theta_{\underline{l}' \underline{k}', n_F(\omega_{\underline{l}'}^-(\underline{k}'))}] \\ g_{\uparrow\uparrow}(\underline{l}\underline{k}) &= \sum_{\underline{l}'} \int_{\text{IBZ}} \frac{d^3 k'}{(2\pi)^3} \mathcal{V}_{\underline{l}\underline{k} + \underline{Q} \underline{l}' \underline{k}'}^{\underline{l}\underline{k} \underline{l}' \underline{k}' + \underline{Q}} \sqrt{\frac{g_{\uparrow\uparrow}(\underline{l}' \underline{k}')}{g_{\uparrow\uparrow}(\underline{l}' \underline{k}')}} \cos \theta_{\underline{l}' \underline{k}'} \sin \theta_{\underline{l}' \underline{k}'} [n_F(\omega_{\underline{l}'}^+(\underline{k}')) - n_F(\omega_{\underline{l}'}^-(\underline{k}'))] \\ g_{\uparrow\downarrow}(\underline{l}\underline{k}) &= \sum_{\underline{l}'} \int_{\text{IBZ}} \frac{d^3 k'}{(2\pi)^3} \mathcal{V}_{\underline{l}\underline{k} + \underline{Q} \underline{l}' \underline{k}' + \underline{Q}}^{\underline{l}\underline{k} + \underline{Q} \underline{l}' \underline{k}' + \underline{Q}} \sqrt{\frac{g_{\uparrow\uparrow}(\underline{l}' \underline{k}')}{g_{\uparrow\uparrow}(\underline{l}' \underline{k}')}} \cos \theta_{\underline{l}' \underline{k}'} \sin \theta_{\underline{l}' \underline{k}'} [r_F(\omega_{\underline{l}'}^+(\underline{k}')) - n_F(\omega_{\underline{l}'}^-(\underline{k}'))] \end{aligned} \quad (C-6)$$

The equations for $g_{\uparrow\uparrow}$, $g_{\uparrow\downarrow}$ may be written more explicitly as follows in section 11-ARPA

$$g_{\uparrow\uparrow}(\mathbf{k}) = \sum_{\mathbf{l}'} \int_{\text{IBZ}} \frac{d^3 \mathbf{k}'}{(2\pi)^3} \mathcal{V}_{\mathbf{k}+\mathbf{Q} \mathbf{l}' \mathbf{k}'}^{\mathbf{l} \mathbf{k}'} \frac{g_{\uparrow\uparrow}(\mathbf{l}' \mathbf{k}')}{[\omega_{\mathbf{l}'}^+(\mathbf{k}') - \omega_{\mathbf{l}'}^-(\mathbf{k}')] } [n_F(\omega_{\mathbf{l}'}^+(\mathbf{k}')) - n_F(\omega_{\mathbf{l}'}^-(\mathbf{k}'))] \quad (\text{C-7})$$

and a similar equation for $g_{\uparrow\downarrow}(\mathbf{k})$.

Lastly, the expression for total energy of this system in HF may be computed using these Green's functions as before. This is seen to be

$$\begin{aligned} \frac{\langle H \rangle}{\Omega_0} = & \sum_{\mathbf{l}} \int_{\text{IBZ}} \frac{d^3 \mathbf{q}}{(2\pi)^3} [(\epsilon_{\mathbf{l}}(\mathbf{q}) \cos^2 \theta_{\mathbf{l}\mathbf{q}} + \epsilon_{\mathbf{l}}(\mathbf{q}+\mathbf{Q}) \sin^2 \theta_{\mathbf{l}\mathbf{q}}) n_F(\omega_{\mathbf{l}}^+(\mathbf{q})) \\ & + (\epsilon_{\mathbf{l}}(\mathbf{q}) \sin^2 \theta_{\mathbf{l}\mathbf{q}} + \epsilon_{\mathbf{l}}(\mathbf{q}+\mathbf{Q}) \cos^2 \theta_{\mathbf{l}\mathbf{q}}) n_F(\omega_{\mathbf{l}}^-(\mathbf{q}))] \\ & - \frac{1}{2} \sum_{\mathbf{l}'} \int_{\text{IBZ}} \int_{\text{IBZ}} \frac{d^3 \mathbf{q} d^3 \mathbf{q}'}{(2\pi)^6} \left\{ \mathcal{V}_{\mathbf{l}' \mathbf{q}' \mathbf{l} \mathbf{q}}^{\mathbf{l}' \mathbf{q}' \mathbf{l} \mathbf{q}} (\cos^2 \theta_{\mathbf{l}' \mathbf{q}'} n_F(\omega_{\mathbf{l}'}^+(\mathbf{q}')) + \right. \\ & \left. + \sin^2 \theta_{\mathbf{l}' \mathbf{q}'} n_F(\omega_{\mathbf{l}'}^-(\mathbf{q}')))(\cos^2 \theta_{\mathbf{l}' \mathbf{k}'} n_F(\omega_{\mathbf{l}'}^+(\mathbf{q}')) + \sin^2 \theta_{\mathbf{l}' \mathbf{k}'} n_F(\omega_{\mathbf{l}'}^-(\mathbf{q}')) \right. \\ & \left. + \mathcal{V}_{\mathbf{l}' \mathbf{q}'+\mathbf{Q} \mathbf{l} \mathbf{q}+\mathbf{Q}}^{\mathbf{l}' \mathbf{q}' \mathbf{l} \mathbf{q}+\mathbf{Q}} (\sin^2 \theta_{\mathbf{l}' \mathbf{k}'} n_F(\omega_{\mathbf{l}'}^+(\mathbf{q}')) + \cos^2 \theta_{\mathbf{l}' \mathbf{k}'} n_F(\omega_{\mathbf{l}'}^-(\mathbf{q}')))(\sin^2 \theta_{\mathbf{l}' \mathbf{q}'} n_F(\omega_{\mathbf{l}'}^+(\mathbf{q}')) + \right. \\ & \left. + \cos^2 \theta_{\mathbf{l}' \mathbf{q}'} n_F(\omega_{\mathbf{l}'}^-(\mathbf{q}')) \right. \\ & \left. + \mathcal{V}_{\mathbf{l}' \mathbf{q}' \mathbf{l} \mathbf{q}+\mathbf{Q}}^{\mathbf{l}' \mathbf{q}' \mathbf{l} \mathbf{q}+\mathbf{Q}} \sqrt{\frac{g_{\uparrow\uparrow}(\mathbf{l}\mathbf{q}) g_{\uparrow\uparrow}(\mathbf{l}' \mathbf{q}')}{g_{\uparrow\uparrow}(\mathbf{l}\mathbf{q}) g_{\uparrow\uparrow}(\mathbf{l}' \mathbf{q}')}} \cos \theta_{\mathbf{l}\mathbf{q}} \sin \theta_{\mathbf{l}\mathbf{q}} \cos \theta_{\mathbf{l}' \mathbf{q}'} \sin \theta_{\mathbf{l}' \mathbf{q}'} \right. \\ & \left. [n_F(\omega_{\mathbf{l}}^+(\mathbf{q})) - n_F(\omega_{\mathbf{l}}^-(\mathbf{q}))][n_F(\omega_{\mathbf{l}'}^+(\mathbf{q}')) - n_F(\omega_{\mathbf{l}'}^-(\mathbf{q}'))] \right. \\ & \left. + \mathcal{V}_{\mathbf{l}' \mathbf{q}' \mathbf{l} \mathbf{q}+\mathbf{Q}}^{\mathbf{l}' \mathbf{q}' \mathbf{l} \mathbf{q}+\mathbf{Q}} \sqrt{\frac{g_{\uparrow\uparrow}(\mathbf{l}\mathbf{q}) g_{\uparrow\uparrow}(\mathbf{l}' \mathbf{q}')}{g_{\uparrow\uparrow}(\mathbf{l}\mathbf{q}) g_{\uparrow\uparrow}(\mathbf{l}' \mathbf{q}')}} \cos \theta_{\mathbf{l}\mathbf{q}} \sin \theta_{\mathbf{l}\mathbf{q}} \cos \theta_{\mathbf{l}' \mathbf{q}'} \sin \theta_{\mathbf{l}' \mathbf{q}'} \right. \\ & \left. [n_F(\omega_{\mathbf{l}}^+(\mathbf{q})) - n_F(\omega_{\mathbf{l}}^-(\mathbf{q}))][n_F(\omega_{\mathbf{l}'}^+(\mathbf{q}')) - n_F(\omega_{\mathbf{l}'}^-(\mathbf{q}'))] \right\} \quad (\text{C-8}) \end{aligned}$$

This generalizes (2.5.26) for Bloch electrons. We may remark that just as for $Q = 0$, the equations for $g_{\uparrow\downarrow}$ and $g_{\downarrow\uparrow}$ are now coupled integral equations. In the above calculation, the Umklapp processes were neglected which implies the neglect of local field corrections and thus broad bands [44]. This formally completes the analysis of SDW for Bloch electrons.

P-STATE INSTABILITY

The solution obtained in Section III-2 was not quite suitable for discussing the P state stability when the Coulomb case for $\xi = 0$ is considered. Here we derive the correct criterion for P state instability. Consider the spin wave equation (3.2.42) in the limit $\omega = 0$, $\xi = 0$ (P state). Then

$$\begin{aligned}
 & - \left(\frac{pq\mu}{m} + \frac{q^2}{2m} \right) \Gamma(p; q) + \left\{ \int \frac{d^3 k}{(2\pi)^3} \mathcal{V}_Y(p-k) [n_F(\omega(k+q)) - n_F(\omega(k))] \right\} \Gamma(p; q) \\
 & = \int \frac{d^3 k}{(2\pi)^3} \mathcal{V}_Y(p-k) [n_F(\omega(k+q)) - n_F(\omega(k))] \Gamma(k; q) \quad (D-1)
 \end{aligned}$$

Now let

$$\begin{aligned}
 \Gamma(p; q) &= \sum_{i, l, m} q^i Y_{lm}(\hat{p}) \Gamma_{lm}^i(p) \\
 \mathcal{V}_Y(p-k) &= \sum_{lm} \frac{2\pi}{pk} Q_l \left(\frac{p^2 + k^2 + \xi^2 k_F^2}{2pk} \right) Y_{lm}(\hat{p}) Y_{lm}^*(\hat{k}) \quad (D-2)
 \end{aligned}$$

$$n_F(\omega(k+q)) - n_F(\omega(k)) = \sum_{i, lm} q^i Y_{lm}(\hat{k}) n_{lm}^i(k)$$

in (D-1) and integrate over \hat{p} . Then we get

$$\begin{aligned}
& - \frac{pq}{m} \left(\frac{4\pi}{3}\right)^{1/2} \sum_i q^i \Gamma_{10}^i(p) + \frac{q^2}{2m} \sum_i q^i \Gamma_{00}^i(p) \\
& + \frac{e^2}{\pi p} \left\{ \sum_{i_2 i_{lm}} \int k dk Q_i \left(\frac{p^2 + k^2 + \xi^2 k_F^2}{2pk} \right) q^{i+i_2} n_{lm}^{i_2}(k) \right\} \Gamma_{lm}^i(p) \\
& = \frac{e^2}{\pi p} \sum_{i_2 i_{lm}} \int k dk Q_0 \left(\frac{p^2 + k^2 + \xi^2 k_F^2}{2pk} \right) q^{i+i_2} n_{lm}^{i_2}(k) \Gamma_{lm}^i(k) \quad (D-3)
\end{aligned}$$

Equating the coefficients of the like powers of q we get since

$$n_{lm}^{(0)} = 0 \quad (D-4)$$

$$\begin{aligned}
& - \frac{p}{m} \left(\frac{4\pi}{3}\right)^{1/2} \Gamma_{10}^{(0)}(p) + \frac{e^2}{\pi p} \left\{ \sum_{lm} \int k dk Q_l \left(\frac{p^2 + k^2 + \xi^2 k_F^2}{2pk} \right) n_{lm}^{(1)}(k) \right\} \Gamma_{lm}^{(0)}(p) \\
& = \frac{e^2}{\pi p} \sum_{lm} \int k dk Q_0 \left(\frac{p^2 + k^2 + \xi^2 k_F^2}{2pk} \right) n_{lm}^{(1)}(k) \Gamma_{lm}^{(0)}(k) \quad (D-5)
\end{aligned}$$

It is easy to prove that

$$n_{lm}^{(1)}(k) = - \left(\frac{4\pi}{3}\right)^{1/2} |\nabla_k \omega(k)| \delta \left(\frac{k_F^2}{2m} - \omega(k) \right) \delta_{l1} \delta_{m0} \quad (D-6)$$

Then (D-5) takes the form

$$\begin{aligned}
& \frac{p}{m} \Gamma_{10}^{(0)}(p) + \frac{e^2}{\pi p} \left\{ \int k dk Q_1 \left(\frac{p^2 + k^2 + \xi^2 k_F^2}{2pk} \right) |\nabla_k \omega(k)| \delta \left(\frac{k_F^2}{2m} - \omega(k) \right) \right\} \Gamma_{10}^{(0)}(k) \\
& = \frac{e^2}{\pi p} \int k dk Q_0 \left(\frac{p^2 + k^2 + \xi^2 k_F^2}{2pk} \right) |\nabla_k \omega(k)| \delta \left(\frac{k_F^2}{2m} - \omega(k) \right) \Gamma_{10}^{(0)}(p) \quad (D-7)
\end{aligned}$$

Let us take $w \sim k^2/2m$ so that one finally gets a condition for nontrivial solution of (D-7) as

$$1 = \frac{\ar_s}{\pi} [\rho_0 (1 + \xi^2/2) - \rho_1 (1 + \xi^2/2)] \quad (D-8)$$

Now,

$$\rho_0(x) - \rho_1(x) = \frac{1}{2} (1-x) \ln \left| \frac{1+x}{1-x} \right| + 1$$

or

$$1 = \frac{\ar_s}{\pi} \left[1 - \frac{\xi^2}{4} \ln \left(1 + \frac{4}{\xi^2} \right) \right].$$

or

$$1 = \frac{\ar_s}{\pi} \left[1 - \frac{\xi^2}{4} \ln \left(1 + \frac{4}{\xi^2} \right) \right] \quad (D-9)$$

Note that this is precisely (2.5.16) when evaluated for $\xi = 0$. For $\xi \rightarrow 0$, this gives the Bloch condition $\ar_s = \pi$. For $\xi \rightarrow \infty$, $\ln \left(1 + \frac{4}{\xi^2} \right) \sim \frac{4}{\xi^2} - \frac{8}{\xi^4}$

and

$$1 = \frac{\ar_s}{\pi} \left[1 - 1 + \frac{2}{\xi^2} \right] = \left(\frac{\ar_s}{\pi \xi^2} \right) 2,$$

but $\ar_s / \pi \xi^2 = \frac{3}{4} \left(\frac{K\theta'}{\epsilon_F} \right)$, so that we get the Stoner criterion $K\theta' / \epsilon_F = \frac{2}{3}$.

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